Conceptual Engineering Product™ 6.2

Reference Guide

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1.1 Data Regression Background

Predictive methods for phase equilibria usually lack a good theory (at least up to now) which can explain the behaviour of dense fluids. From this point of view, the engineer responsible for the final design of separation equipment would eventually have to "fit" some empirical data to a convenient model, in order to supplement the model's predictions to an acceptable accuracy level. Unfortunately, there are no sharp and easy rules to follow when fitting data to a thermodynamic model. A combination of experience, theoretical knowledge, and common sense is necessary.

Optimization as a Tool for Data Fitting

Although several statistical techniques can be used to fit specific parameters to a given thermodynamic model, such as the *Maximum Likelihood Method* (Anderson et.al., 1978[9]; Press et.al., 1986[119]). It was found through experience that a simple least squares function coupled with a robust optimization algorithm combines flexibility with a reasonable computational speed.

The problem is approached as follows:

$$Minimize\ f = \sum_{i=1}^{No\ of\ Points} \sigma_i^{model}(g_i^{model}(\bar{x}) - g_i^{experimental}) \qquad (1.1)$$

where: g_i^{model} *= the value of a property predicted by the model*

$g_i^{experimental}$ *= the actual measured value for the point i*

$\bar{x}$ *= the vector of parameters which can be manipulated in the thermodynamic model (usually the kij's for an equation of state and the aij's for an activity model)*

σ_i *= the weight for a specific point used to distort the data fit in a convenient way*

Refer to **Section 1.1.2 - Weighting** for more information about *weight*.

This representation has the advantage of allowing the use of any convenient optimization method to manipulate the vector. The algorithm used in regression module is the Powell optimization method (Press et. al., 1986[119]; Edgar et. al., 1986[40]).

This particular optimization method was found to be the most reliable for a rather restrictive class of problems, i.e., VLE and LLE problems using very specialized functions.

By no means should the Powell optimization method be judged as the "most" efficient method for general problems. Phase equilibria teaches us how important it is to be pragmatic and not to overemphasize (or under emphasize) the performance of a given thermodynamic model. The very same lesson applies to optimization techniques.

1.1.1 Basic Thermodynamic Framework

In order to appreciate how the parameters in thermodynamic models are regressed using experimental data, a good understanding of the basic thermodynamic equations as well as knowledge of how the data was obtained from the laboratory or literature is required.

The equilibrium equations used in DISTIL are:

VLE: equation of state approach	$y_i \phi_i^V(T, P, \bar{y}) = x_i \phi_i^L(T, P, \bar{x})$	(1.2)
VLE: activity coefficient approach	$y_i \phi_i^V(T, P, \bar{y}) P = x_i \gamma_i^L(T, \bar{x}) f_i^\circ$	(1.3)
LLE: equation of state approach	$x^{\mathrm{I}} \phi_i^{\mathrm{I}}(T, P, \bar{x}^{\mathrm{I}}) = x^{\mathrm{II}} \phi_i^{\mathrm{II}}(T, P, \bar{x}^{\mathrm{II}})$	(1.4)
LLE: activity coefficient approach	$x^{\mathrm{I}} \gamma_i^{\mathrm{I}}(T, \bar{x}^{\mathrm{I}}) = x^{\mathrm{II}} \gamma_i^{\mathrm{II}}(T, \bar{x}^{\mathrm{II}})$	(1.5)

When thermodynamic models are used to calculate activity or fugacity coefficients in the above thermodynamic equilibrium equations, the model parameters are related to the activity and fugacity coefficients. A mathematical method of minimizing the error between the measured and calculated values can be devised by varying the model parameters until the minimum error is reached.

Thus, (theoretically) the most "correct" coefficients representing the behaviour of a binary mixture could be calculated for a given thermodynamic model. However, this is not without ambiguity due to two main reasons. First, the experimental data are subject to experimental errors which preclude the calculation of unique, meaningful coefficients. Second, the coefficients for the thermodynamic models are dependent on the method by which the data reduction is performed (since they are only approximate representations of the mixture behaviour subject to rather arbitrary assumptions). For instance, if the data is regressed to minimize the deviations with respect to the activity coefficients, the obtained interaction parameters will be different than the ones obtained from data optimized with respect to the relative volatility. This is due in part to the inadequacies of the thermodynamic models to accurately calculate the fugacity and activity coefficient. Until better theories become available, there will always be some ambiguity associated with the optimization of the interaction parameters.

1.1.2 Weighting

When regressing, it is sometimes necessary to "distort" the fit in order to better represent the behaviour of a specific region that is important for the process.

Consider an azeotropic system. Suppose that when the data fit is performed, the azeotropic point was not properly represented. Since the azeotropic point represents a stiff thermodynamic barrier for the separation of the mixture by distillation, it is important to ensure that the azeotrope is well represented. The azeotropic region can be better represented by weighting the azeotropic point(s) heavily and check the fit again to see how badly the non-azeotropic data points were “damaged”. If a reasonable fit is still observed, then the weighting scheme is acceptable. It is preferable to be one or two degrees off, or to be conservative in one or two theoretical trays, than to design an impossible process.

1.1.3 Equations & Shapes used in Regression

DISTIL selects a default equation for regression purposes depending on the property you have selected. The following table lists the temperature dependent property, the equation, and the regressed coefficients.

Temperature Dependent Property	Equation	Shape/Exponent	
		X	Y
Solid Density	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Liquid Density	$Y = \frac{a}{b^{\left(1-\frac{X}{c}\right)^d}}$	0/1	0/1
Vapour Pressure	$Y = a + \frac{b}{X+c} + d\ln(X) + eX^f$	1/1	6/1
Sublimation Pressure	$Y = a + \frac{b}{X} + c\ln(X) + dX^e$	0/1	0/1
Enthalpy of Vapourization	$Y = \ln(a) + \ln(1-X)(b + cX + dX + eX)$	0/1	1/1
Solid Heat Capacity	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Liquid Heat Capacity	$Y = a + bX + cX^2 + dX^3 + eX^4$	n/a	n/a
Ideal Gas Enthalpy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	6/1
Second Virial Coefficient	*Dippr Second Virial Coefficient Function*	0/1	6/1
Liquid Viscosity	$Y = a + \frac{b}{X} + c\ln(X) + dX^e$	0/1	0/1
Gas Viscosity	$Y = \frac{aX^b}{\left(c + \frac{d}{X} + \frac{e}{X^2}\right)}$	0/1	0/1
Liquid Thermal Conductivity	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Gas Thermal Conductivity	$Y = \frac{aX^b}{\left(c + \frac{d}{X} + \frac{e}{X^2}\right)}$	0/1	0/1
Gas Liquid Surface Tension	$Y = \ln(a) + \ln(1-X)(b + cX + dX^2 + eX^3)$	0/1	0/1
PRMathias Copeman	$Y = \ln(a) + \ln(1-X)(b + cX + dX^2 + eX^3)$	0/1	0/1

Temperature Dependent Property	Equation	Shape/Exponent	
		X	Y
Ideal Gas Gibbs Free Energy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Gas Density	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Solid Thermal Conductivity	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
K Value1	$Y = a + \frac{b}{X} + \frac{c}{X^2} + \frac{d}{X^3} + \frac{e}{X^4}$	0/1	27/1
K Value2	$Y = a + \frac{b}{X} + \frac{c}{X^2} + \frac{d}{X^3} + \frac{e}{X^4}$	0/1	27/1
Separation Factor	$Y = a + \frac{b}{X} + \frac{c}{X^2} + \frac{d}{X^3} + \frac{e}{X^4}$	0/1	27/1
Solid Enthalpy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Liquid Enthalpy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Gas Enthalpy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Solid Entropy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Liquid Entropy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Gas Entropy	$Y = a + bX + cX^2 + dX^3 + eX^4$	0/1	0/1
Gas Heat Capacity	$Y = a + b\left\{\frac{c}{X\sinh\left(\frac{c}{X}\right)}\right\}^2 + d\left\{\frac{e}{X\cosh\left(\frac{e}{X}\right)}\right\}^2$	0/1	0/1

If you have data for property, *y*, which is dependent on some value *x* and you want to model *y* using an equation *F(x)*, then the following applies:

$$y = F(x) \tag{1.6}$$

The relationship being studied, however, might be more complicated. You can define shape functions for the *x* and *y* variables so that **Equation (1.6)** becomes:

$$Y(y) = F(X(x)) \tag{1.7}$$

where: X, Y = the shape functions for the variables x and y

In order to define a variables shape function, you must input two pieces of information. The table below is the *Shape Function Code* table which lists the various shapes, along with the corresponding code.

Shape Code	Shape Function	Shape Code	Shape Function
0	y^{exp}	12	$(sin(y))^{exp}$
1	$(y/Tc)^{exp}$	13	$(cos(y))^{exp}$
2	$(1\text{-}y/Tc)^{exp}$	14	$(tan(y))^{exp}$
3	$(log(y))^{exp}$	15	$(sin(y/Tc))^{exp}$
4	$(log(y/Tc))^{exp}$	16	$(cos(y/Tc))^{exp}$
5	$(log(1\text{-}y/Tc))^{exp}$	17	$(tan(y/Tc))^{exp}$
6	$(ln(y))^{exp}$	18	$(sin(1\text{-}y/Tc))^{exp}$
7	$(ln(y/Tc))^{exp}$	19	$(cos(1\text{-}y/Tc))^{exp}$
8	$(ln(1\text{-}y/Tc))^{exp}$	20	$(tan(1\text{-}y/Tc))^{exp}$
9	$(e^{y})^{exp}$	21	$(1\text{-}y)^{exp}$
10	$(e^{(y/Tc)})^{exp}$	22	$(1\text{-}y/Tc)^{exp}$
11	$(e^{(1-y/Tc)})^{exp}$		

You can enter the *Shape Code* and *Exponent* associated with either the X or Y shape functions in the Pure Component Regression.

1.1.4 Herrington Consistency Test Equations

The Herrington Consistency test (Gmehling & Onken, 1977[54]) is based on the Gibbs-Duhem equation:

$$\frac{\Delta H}{RT^2}dT - \frac{\Delta V}{RT}dP + \sum x_i d(\ln\gamma_i) = 0 \tag{1.8}$$

Using the assumption of low or moderate pressures, the consistency test takes the following forms for binary systems:

$$x_1 d(\ln\gamma_1) + x_2 d(\ln\gamma_2) = 0 \qquad T\ constant \tag{1.9}$$

$$x_1 d(\ln\gamma_1) + x_2 d(\ln\gamma_2) + \frac{\Delta H}{RT^2}dT = 0 \qquad P\ constant \tag{1.10}$$

The equation of the differential of excess Gibbs energy is:

$$d\left(\frac{G^E}{RT}\right) = x_1 d\ln\gamma_1 + x_2 d\ln\gamma_2 + \ln\gamma_1 dx_1 - \ln\gamma_2 dx_1 \tag{1.11}$$

Combining and integrating:

$$\int_0^1 \ln\frac{\gamma_1}{\gamma_2}dx_1 = 0 \qquad T\ \ constant \tag{1.12}$$

$$\int_0^1 \ln\frac{\gamma_1}{\gamma_2}dx_1 + \int_{T_o}^{T_1} \frac{\Delta H}{RT^2}dT = 0 \qquad P\ \ constant \tag{1.13}$$

since $\int_0^1 d\left(\frac{G^E}{RT}\right) = 0$.

Since the area under the curve is equal to zero, the area above the x axis is equal to the area below the x axis. However, due to experimental uncertainty, the following can be defined:

$$D = 100\left|\frac{(A-B)}{(A+B)}\right| \tag{1.14}$$

where: A = *the area above the x axis*

B = *the area below the x axis*

For isobaric data, Herrington proposed the following semi-empirical relation:

$$J = 150\left|\frac{\Delta T_{max}}{T_{min}}\right| \tag{1.15}$$

where: T_{min} = *the minimum boiling point temperature for the system*

ΔT_{max} = *the maximum temperature difference in the system*

If $D \leq 5\%$, the data are considered to be consistent (T constant).

If $D - J \leq 10\%$, the data are considered to be consistent (P constant).

2 Azeotropic Distillation - Engineering Insights

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2.1 Introduction

The information presented in this chapter will help you understand the system and governing physics behind azeotropic distillation. Common and important terms associated to azeotropic distillation will be defined, as well as the basic theory that builds the foundation for the procedures used in generating column sequences and column designs.

2.2 Azeotropes

Some mixtures will boil at constant temperature producing a vapour with identical composition to the liquid. This phenomenon is called azeotropism.

So some mixtures cannot be separated (into pure component) using simple distillation because of azeotropism. The liquid mixture in the distillation column will boil to vapour, but the composition of the vapour remains the same as the liquid composition. Thus no separation has occur.

The composition, pressure, and temperature point where azeotropism occur is referred to as an azeotrope point or singular point. There are three types of azeotropes: binary azeotrope, azeotropes occurring in a three or more components mixture, and heterogeneous azeotropes.

2.2.1 Bifurcation Theory

This section discusses the application of homotopy continuation for finding multi-component azeotropes (Fidkowski et. al., 1993[44]).

At an azeotropic point, the compositions of the liquid and vapour phases at equilibrium are the same. This can be represented as:

$$y_i - x_i = 0 \qquad i = 1, 2, \ldots, c-1 \tag{2.1}$$

Equation (2.1) is subject to the vapour-liquid equilibrium constraints and mole fraction constraints. It is difficult to solve this equation for a multi-component system, as it is a non-linear constrained problem with multiple solutions. There will be at least as many solutions as there are components, as well as any additional solutions represent azeotropes in the system.

The homotopy method discussed here is used to find all of the roots of the set of non-linear equations which describe azeotropic conditions in a multi-component system.

Raoult's law gives the ideal equilibrium relationship for a component *i*:

$$y_i^{id} = \frac{p_i^s}{P} x_i \tag{2.2}$$

Raoult's law is modified for models which use activity and fugacity coefficients to describe non-ideal behaviour:

$$y_i = \frac{\gamma_i p_i^s}{\phi_i P} x_i \tag{2.3}$$

An "artificial" equilibrium relation can be defined which includes both the ideal and non-ideal relations in its formulation:

$$y_i = \left[(1-t) + t\frac{\gamma_i}{\phi_i}\right]\frac{p_i^s}{P}x_i \qquad (2.4)$$

where: t = the homotopy parameter

When $t = 0$, this equilibrium relation simplifies to the Raoult's Law and when $t = 1$, it represents the actual non-ideal solution.

The azeotrope-finding procedure involves increasing t from 0 to 1 and finding *bifurcation* points at existing branches.

When a *singularity* is encountered on the branch (that is, a value of t is found for which there is a non-unique solution), it can be shown to be a bifurcation point with two branches of solutions. Thus, when there is a new path, it will always branch from the pure component line; this results in a binary (two-component) azeotrope. The azeotropic conditions can be determined by extending the new branch to the limiting condition of the homotopy parameter ($t = 1$). If there is a bifurcation in this branch, the new path will produce a ternary azeotrope. Ternary azeotropes are possible only for systems which have three or more components. This line of reasoning can be extended to systems with any number of components.

From the bifurcation diagram, the temperature of the azeotropes can be read at the point where the homotopy parameter is equal to 1.0.

2.2.2 Types of Azeotropes

DISTIL has a rigorous algorithm that can accurately calculate all of the azeotropes in a multi-component system (predicted by the property package and interaction parameters).

Previously mentioned, there are three type of azeotropes. The following section will describe each type of azeotrope in detail.

Two Component Mixture

For a binary system, there are two types of azeotropes:

Azeotrope	Description
Unstable	Characterized by a minimum boiling temperature at constant pressure. The mixture at azeotropic composition boils at a temperature lower than the individual components that make up the mixture.
Stable	Characterized by a maximum boiling temperature at constant pressure. The mixture at azeotropic composition boils at a temperature higher than the individual components that make up the mixture.

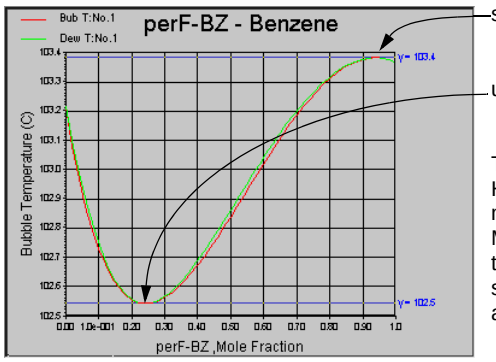
Most binary azeotropic systems have just one minimum or maximum-boiling temperature azeotrope. You cannot have binary azeotrope with intermediate boiling temperature.

Other binary systems with two azeotropes:

- Methyl acetate & Butylene-1,2-oxide
- Diethylamine & Methanol

There are only a few known binary systems with multiple azeotropes (e.g., Hexafluorobenzene and Benzene, which has minimum and maximum boiling azeotropes).

Figure 2.1



TXY Diagram for Hexafluorobenzene & Benzene mixture at 2 atm (NRTL Ideal). Minimum and maximum boiling temperature azeotropes can be seen at temperatures of 102.5°C and 103.4°C, respectively.

Three or More Component Mixture

For systems with three or more components, there are three types of azeotropes and pure components (or singular points of RCM):

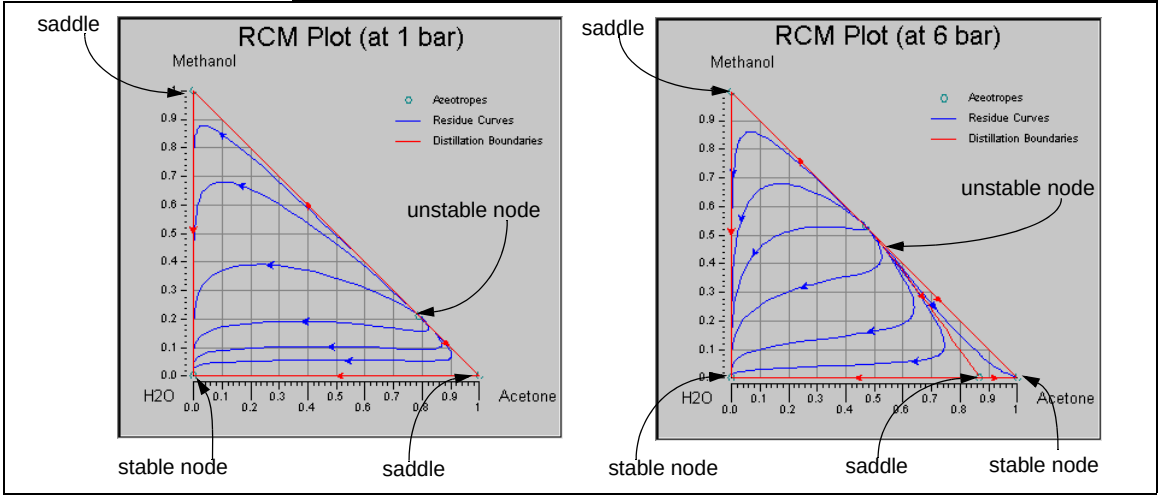
The vast majority of azeotropes are minimum boiling azeotropes; maximum boiling azeotropes are not as common.

Azeotrope	Description
Unstable node	This is a minimum boiling azeotrope. This is called an unstable node because all residue curves in the node's vicinity move away from this stationary point. In a distillation column with infinite reflux, this is the composition that can be taken from the distillate.
Stable node	This is a maximum boiling point azeotrope. It is called a stable node because all residue curves in the node's vicinity converge to that stationary point. In a distillation column with infinite reflux, this is the composition that can be taken from the bottoms.
Saddle	This stationary point has a bubble point, which is neither a minimum or maximum boiling temperature at a specific pressure. Residue curves approach but do not pass through the saddles.

The type of an azeotrope in a mixture depends on the interactions between all components in a specific mixture and given conditions (e.g., temperature, pressure) and not on the behaviour of the components taken separately.

An example of this would be to compare the Acetone-Methanol-Water system at different pressure. At 1 bar, the Acetone is a saddle and the mixture contains one azeotrope. At 6 bar, the Acetone is a stable node and the mixture contains two azeotrope.

Figure 2.2



Another example would be to compare two mixtures: n-Butane, n-Pentane & n-Hexane (mixture 1), and n-Pentane, n-Hexane & n-Heptane (mixture 2). At 1 bar, n-Pentane in mixture 1 is a saddle. At 1 bar, n-Pentane in mixture 2 is an unstable node.

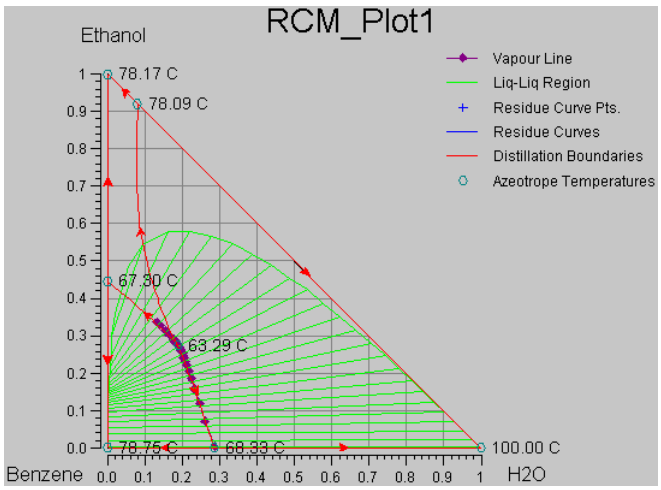
Heterogeneous Azeotropes

A heterogeneous azeotrope is a mixture that, when boiled, produces a vapour with the same composition as the bulk liquid, but the liquid itself is unstable, splitting into two liquid phases. DISTIL is capable of predicting multiple liquid phases.

Heterogeneous azeotropes are common in industry (e.g., in alcohol dehydration process). In dehydration processes, a third component is added (called entrainer) and it forms a low boiling azeotrope with the other components in the mixture. This azeotrope goes to the top of the distillation column, thus allowing the column to produce the desired product at the bottom.

Common entrainers for dehydration of alcohols by heterogeneous azeotropic distillation are benzene and cyclohexane.

Figure 2.3



A common misconception is that equations of state cannot predict azeotropes. Another misconception is that hydrocarbons do not form

azeotropes. On the contrary, there are many azeotropes between paraffins and olefins, as well as aromatic and cyclo-paraffins.

2.2.3 Singular Points

For example, in the mixture n-Pentane, n-Hexane and n-Heptane at 1 bar, there are no azeotropes, but each pure component is a singular point: pure n-Pentane is an unstable node, pure n-Hexane is a saddle and pure n-Heptane is a stable node. So the mixture has three singular points.

Pure components and azeotropes of RCM are singular points or stationary points.

For a mixture, there are at least as many singular points as there are pure components, and every azeotrope adds an additional singular point. For example, a three-component mixture with two azeotropes has five singular points.

Systems with different numbers of azeotropes are discussed in **Section 2.3.3 - Distillation Boundaries (DB)**.

Consistency Test

For more information regarding the consistency test, refer to Wasylkiewicz et. al. (1999, p. 4907)[166].

The relationship among different type of singular points is described by the topological constraint. The topological consistency of the calculated azeotropes can be checked from the following topological constraint (Zharov and Serafimov, 1975[177]):

$$\sum_{k=1}^{c} 2^k (N_k^+ + S_k^+ - N_k^- - S_k^-) = (-1)^{c-1} + 1 \qquad (2.5)$$

where: N_k^+, S_k^+ = *numbers of k-component nodes and saddles with index +1*

N_k^-, S_k^- = *corresponding singular points with an index of -1*

The index is related to the number of negative eigenvalues of the Jacobian used to determine the type of azeotropic points.

If the topological constraint status is unsatisfied, the solution is not correct. This could mean that the component data or property package are unreliable.

If the topological constraint status is satisfied, this does not necessarily prove that the solution is correct, but it allows you to place more confidence in the results.

2.3 Residue Curve Map (RCM)

For more information regarding the theory of residue curve map, refer to Wasylkiewicz et. al. (1999)[169].

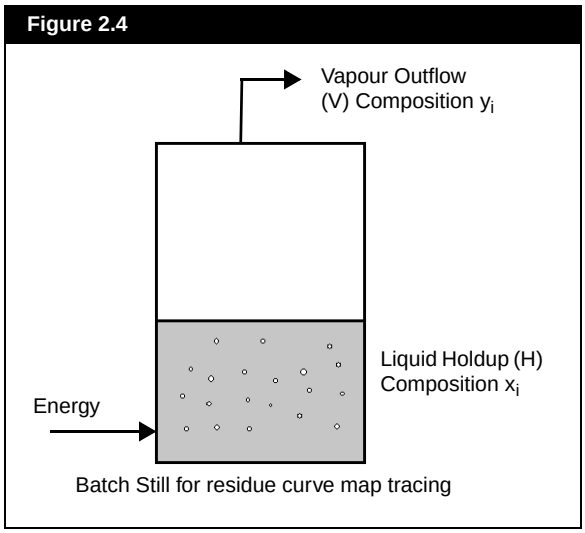
Residue curve maps describe in a rich and intuitive way the distillation paths in a distillation tower. In addition, combined with azeotrope calculation capabilities, distillation boundaries can be displayed, allowing you to determine the feasibility of a proposed separation at a glance.

A residue curve is the path traced in the composition space plot that represent the change in composition of the residue over time in a batch distillation.

2.3.1 Calculation

The figure below is the batch still model that is used to generate the residue curve maps.

Figure 2.4



The mass balance of the simple distillation process in the figure above can be described by the following equations:

$$\frac{dH}{dt} = -V \tag{2.6}$$

$$\frac{d(Hx_i)}{dt} = -Vy_i \tag{2.7}$$

where: H = *the liquid holdup*

t = *the time*

V = *the vapour outflow*

x_i = *the liquid composition of component i*

y_i = *the vapour composition of component i*

If the differential in **Equation (2.7)** is expanded and combine d with the $\frac{dH}{dt}$ term from **Equation (2.6)**, the following is obtained:

$$H\frac{d(x_i)}{dt} + x_i\frac{d(H)}{dt} = -Vy_i \tag{2.8}$$

$$\frac{d(x_i)}{dt} = \frac{V}{H}(x_i - y_i) \tag{2.9}$$

Using the same transformation as Doherty and Perkins for homogeneous systems (Doherty and Perkins, 1978[32]):

$$H\frac{dx_i}{d\xi} = x_i - y_i \tag{2.10}$$

where: ξ = *the "warped" time going from 0 to* $+\infty$

When $t = 0$, $\xi = 0$

When $t = t_d$, $\xi = +\infty$

t_d = *the time necessary for the pot to dry up*

The basic algorithm for the residue curve map tracing is as follows:

1. Set initial values for x and P.
2. Calculate T and y using a rigorous bubble point procedure.
3. Integrate **Equation (2.10)** for one warped time step; i.e., calculate x at $\xi = \xi^{\circ} + \Delta\xi$ and go back to step #2.
4. Continue integration until a singular point is reached (until composition does not change).

Mathematically, you can also go from 0 to $-\infty$.

2.3.2 Physical Significance

The analysis of the structure of the residue curve maps has been subjected to extensive studies by Doherty and Perkins (1978)[32], Van Dongen and Doherty (1984)[158] and Pham and Doherty (1990)[118]. The basic result from these analyses is that only nodes and saddles can occur in residue curve maps.

- Homogeneous azeotropes can be stable nodes (high boiling azeotropes), unstable nodes (low boiling azeotropes), or saddles (medium boiling azeotropes).
- Heterogeneous azeotropes can be either unstable nodes or saddles, **but** they cannot be stable nodes (in another words, they cannot be high boiling azeotropes).

Residue curves cannot cross each other or go beyond singular points.

An interesting characteristic of the residue curve is that, although being the solution of a differential equation in "warped time", it is a new thermodynamic property of the system, being uniquely defined at a given pressure and starting composition x_i^{o}. Since the residue curve describes the actual physical process of boiling off a mixture, it always advances in the direction of increasing temperature in the system. The heavier boiling components in the system are being concentrated in the still. An azeotrope can be detected in the residue curve as a fixed point, which boils at fixed composition and temperature.

2.3.3 Distillation Boundaries (DB)

Distillation boundaries separate distillation regions that cannot be crossed by simple stage-by-stage distillation. A distillation region is a collection of all residue curves that start at the same unstable node and end at the same stable node. For a ternary mixture, a distillation boundary is a dividing line between two families of residue curves.

To summarize, a residue curve is the composition path of the liquid phase in an isobaric open evaporation. The equations describing the process are analogous to the equations describing a batch distillation and were discussed by Doherty and Perkins (1978)[32]. A residue curve map has the following characteristics:

- The residue curves always point in the direction of increasing temperature.
- Pure components and azeotropes are singular points in the map.
- Azeotropes give rise to boundaries in the composition space, signalling different qualitative behaviour depending on where a mixture to be separated is in the composition space.
- The residue curve map displays distillation boundaries and distillation regions in the component space.
- Residue curves are equivalent to the composition profiles in a packed distillation tower at constant pressure and infinite reflux.

An important benefit that a residue curve map provides is that it is a qualitative description of the composition profile that would be observed in an actual distillation tower operating at total reflux.

2.3.4 Examples

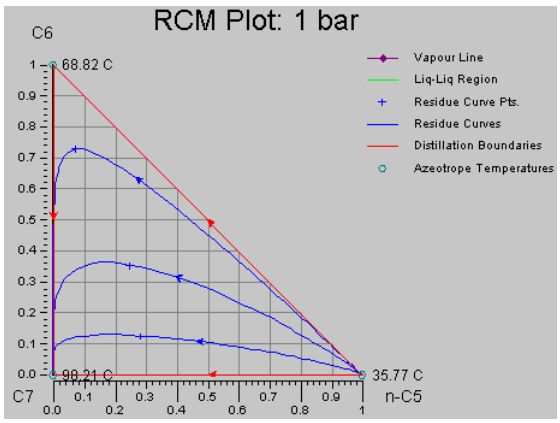
The residue curve maps for a few common systems are shown in the following sections.

No Azeotropes: n-C5, n-C6, and n-C7 at 1 bar

The property package for the RCM is NRTL-Ideal.

The residue curve map for an almost ideal system of n-Pentane, n-Hexane and n-Heptane at 1 bar is shown in the figure below.

Figure 2.5



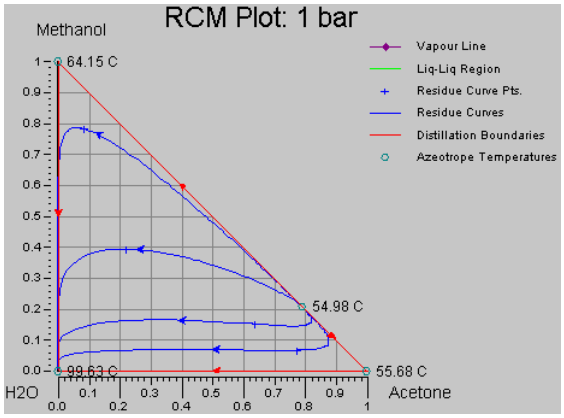
Just by looking at the RCM plot, you can notice that there are no distillation boundaries. The n-Pentane is an unstable node (minimum boiling), n-Hexane is a saddle (intermediate boiling), and n-Heptane is a stable node (maximum boiling). The residue curves show the path traced in the composition space by the liquid in the batch distillation still. The arrows point in the direction of increasing boiling temperature.

One Azeotrope: Acetone, Methanol, and Water at 1 bar

The property package for the RCM is UNIQUAC-Ideal.

Now let us examine a ternary mixture with one binary azeotrope. The residue curve map for Acetone, Methanol, and Water at 1 bar is shown in the figure below.

Figure 2.6



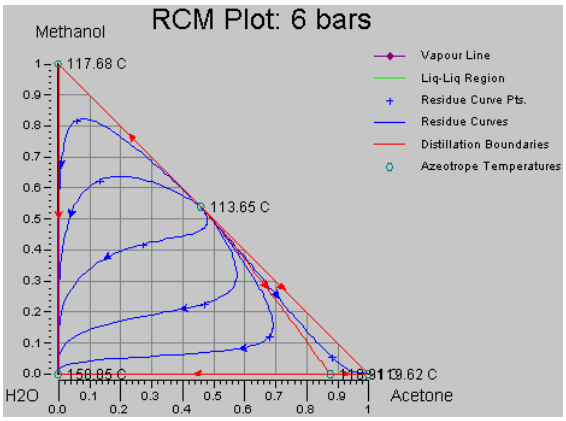
The azeotrope between Acetone and Methanol is shown in the map. It has a big influence on the behaviour of the residue curves. For a feed located in the upper part of the map, you can reach the Methanol saddle (i.e., low water composition). Whereas for a feed in the lower part of the map (i.e., high water composition), you cannot approach the Methanol saddle point.

Two Azeotropes: Acetone, Methanol, and Water at 6 bar

The property package for the RCM is UNIQUAC-Ideal.

The figure below shows a change in the residue curve map when the pressure of the Acetone-Methanol-Water system is changed from 1 to 6 bars.

Figure 2.7



A new azeotrope between Acetone and Water appears and a distillation boundary can be observed. Also notice that the azeotrope between Acetone and Methanol has moved. The appearance of the distillation boundary gives rise to two distillation regions in the composition space. The products from a simple distillation column cannot be in different regions. A bifurcation pressure, which is defined as the pressure at which a new azeotrope appears or disappears, is around 3 bar for the Acetone and Water azeotrope.

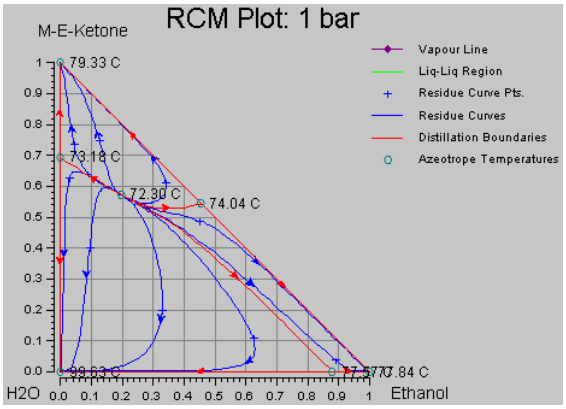
Multiple Azeotropes

Systems with more azeotropes will, in general, result in more complex residue curve maps.

The property package for the RCM is Wilson-Ideal.

For example, the figure below shows the residue curve map for a mixture of Ethanol, Methyl-Ethyl-Ketone, and Water at 1 bar.

Figure 2.8

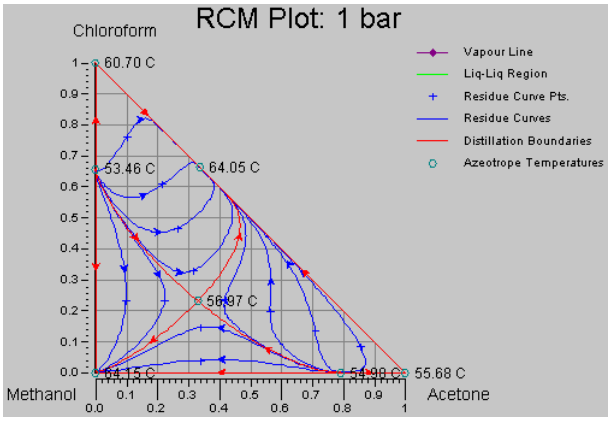


There are three binary azeotropes and one ternary azeotrope, giving a residue curve map with three distillation regions.

The property package for the RCM is Wilson-Ideal Gas.

Another example is a mixture of Acetone, Chloroform, and Methanol at 1 bar. The RCM contains four distillation regions.

Figure 2.9



2.3.5 Use of RCM and DB

The RCM and DB define a system topology (i.e., azeotropes, singular points, node types, and distillation boundary) that depends only on the operating pressure. The system topology provides useful insights about what separation is feasible using simple distillation.

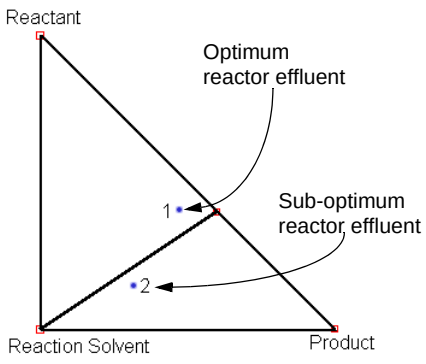
The following example illustrates how the system topology can be used at the process synthesis level to improve design efficiency of a separation system.

Example

A chemist in a Reseach & Developement lab of a speciality chemical company is developing a new catalyst to optimise selectivity and yield. The chemist generates an optimum reactor design and asks a process engineer to look at it from the separation point of view to obtain pure product stream.

The process engineer can use the RCM plot below and the system topology to quickly evaluate what separation is feasible and what is not.

Figure 2.10



The reactor effluent of the optimum reactor design on the RCM above shows that product separation requires crossing the distillation boundary and hence more expensive separation system is required. Refer to point 1 in **Figure 2.10**.

Based on the previous RCM plot, the process engineer can explain the overall process economics to the chemist. The process engineer can also asks the chemist to design a catalyst and a condition, such that the reactor effluent is on the Product side of the distillation boundary.

It was found that with a little modification in the catalyst temperature and a small sacrifice in the selectivity of the system, a reactor effluent on the Product side of the distillation boundary is possible. Refer to point 2 in **Figure 2.10**. The sub-optimum reactor effluent option simplifies the separation system greatly.

Thus at the early design stage, the RCM plot not only helps in making important process decisions, but also provides the direction for improving the system.

2.4 Distillation Region Diagram

The Distillation Region Diagram (DRD) represents all possible topologies (azeotropes, singular points, node types, and temperatures) for a ternary system.

The DRD are extremely useful when the VLE data of the components is not available.

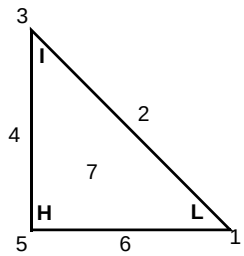
The DRD provides complete information of the distillation boundaries when you provide the information about all the azeotropes and the temperatures of all singular points (i.e., azeotropes and pure products). The DRD is also very valuable in evaluating the consistency of lab data and evaluating whether more data is necessary.

For example, if the lab data shows that no binary azeotrope is present, but a ternary azeotrope is present. The DRD can be used to confirm that the data is inconsistent. Either the existent of the ternary azeotrope in the lab data is incorrect, or one or more binary azeotropes were missed.

Remember, the DRD is limited to ternary system only.

The DRD generates a temperature profile and a map number when the temperatures of all the singular points are provided. This map number is extremely useful in sequence synthesis, please refer to **Perry's Chemical Engineers' Handbook** (7th edition)[108] for more information.

2.4.1 Temperature Profile



Temperature Profile Diagram
L: Low Boiling Component
H: High Boiling Component
I: Intermediate Component

Another way to represent and reproduce a DRD is by its temperature profile sequence. For ternary systems containing no more than one ternary azeotrope, and no more than one binary azeotrope between each pair of components, 125 types of DRD are mathematically possible.

Here is the procedure that defines the Temperature Profile Sequence:

- Classify a system by writing down each position number in ascending order of boiling points, using the **Temperature Profile Diagram**.

A position number is not considered if there is no azeotrope at that position. Each temperature profile will have a minimum of three numbers and a maximum of seven numbers. Positions 1,3 and 5 indicate the pure components in order of decreasing volatility. Positions 2, 4 and 6 are binary azeotropes situated between the pure components. Position 7 is a ternary azeotrope. For more information regarding Temperature Profile Sequences, refer to page 13-58 of the **Perry's Chemical Engineers' Handbook** (seventh edition)[108].

DRD are particularly useful in determining the implications of possibly unknown ternary saddle azeotropes by postulating position 7 at interior positions in the temperature profile.

2.5 Azeotrope Analysis

The behaviour of the azeotropes depends strongly on the pressure of the system. Many azeotropes appear/disappear or their compositions vary as the pressure changes. Hence, it is extremely important to see how topology is affected by the pressure before one looks at the sequence generation.

Pressure analysis is helpful in deciding the operating pressure of the separation system and evaluating the potential for pressure saving distillation designs.

DISTIL employs pressure continuation method to evaluate the pressure sensitivity of the possible azeotropes in the separation system. The following example illustrates the ideas mentioned above.

Example

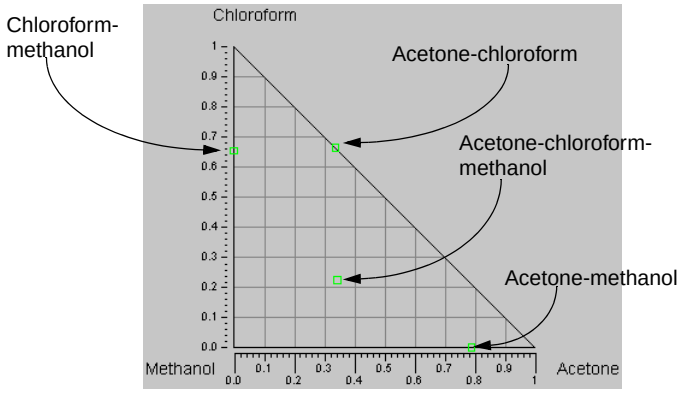
Consider the following fluid package, components, and pressure range:

Fluid Package	Components	Pressure Range
NRTL-Ideal Gas	Acetone, Chloroform, and Methanol	100 kPa to 2500 kPa

Three binary azeotropes and one ternary azeotropes.

At 100 kPa there are four azeotropes: acetone-chloroform, acetone-methanol, chloroform-methanol, and acetone-chloroform-methanol.

Figure 2.11

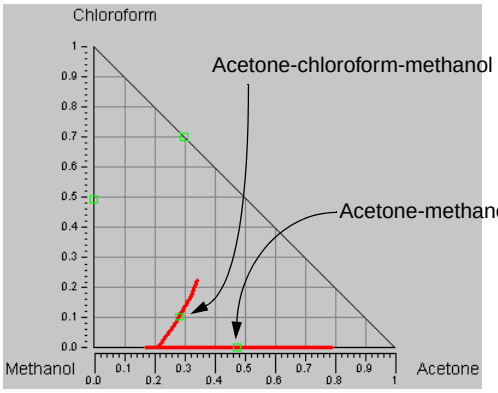


As the pressure increases, the amount of chloroform in the ternary azeotrope composition decreases.

Notice as the pressure increases the ternary azeotrope moves closer to the acetone-methanol binary azeotrope.

Figure 2.12

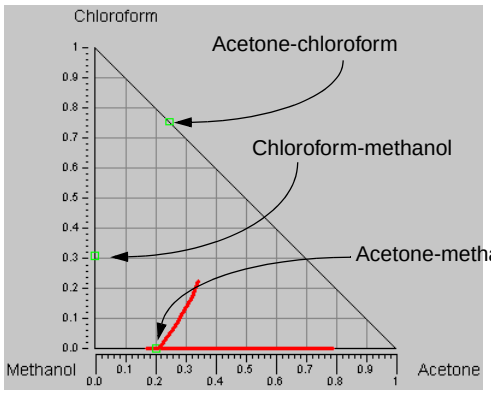
Mixture at 580 kPa



At 2020 kPa, the ternary azeotrope (acetone-chloroform-methanol) point has just about touched/joined the binary azeotrope (acetone-methanol). If you checked the composition of the ternary azeotrope, the chloroform mole value has been reduced to about $2.231*10^{-3}$ which is very close to zero.

At 2140 kPa, the ternary azeotrope has disappeared and there are only three binary azeotropes in the mixture.

Figure 2.13



So by increasing the pressure to a certain amount, you can reduce the number of azeotropes and thus reduce the number of boundaries that prevent you from separating the mixture.

In conclusion, it is important to perform azeotrope analysis at different pressure range, because it could mean the difference between being able or not being able to split the mixture in the column.

3 Azeotropic Distillation - Sequence Generation

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3.1 Introduction

The engineering insights generated in the previous chapter are used to setup and solve a separation sequencing problem.

- The information about azeotropes and singular points is used to define the distillation boundaries and regions in multi-component system.
- The type of solvent (if required) is screened by examining Residue Curve Map system topology.
- The results of pressure analysis is used to define the number of pressure levels and their values.

This chapter will describe the extension of the graphical methods used in designing distillation columns for separation of binary and ternary mixtures (in the Column Design views) to mixtures of any number of components. Geometric methods used for designing distillation systems focused primarily on two and three component systems. It is not possible to use graphical techniques for more than four components. The Column Sequencing operation uses an equation based (non-visual) methodology which has been extended to any number of components. With Column Sequencing, a matrix formulation is used to embed the information contained in a Residue Curve Map.

Using the Column Sequencing, you can calculate azeotropes in the system, determine the structure of distillation regions, and assess the feasibility of separation of multi-component mixtures.

Column Sequencing generates numerous feasible distillation sequences that separate azeotropic and non-azeotropic mixtures into pure components and/or azeotropes. Separation of a specified feed is achieved using a series of simple distillation columns operating at pre-specified pressure levels.

Column Sequencing provides the following information for systems with any number of components:

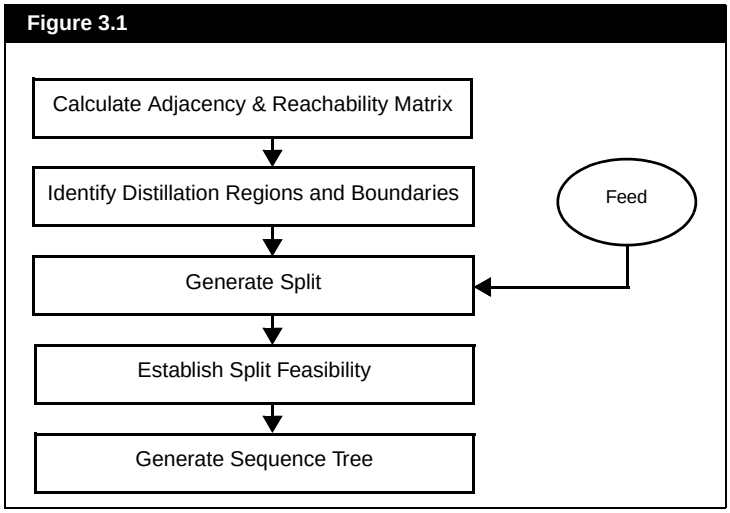
- All azeotropes in the system predicted by the VLE model.
- The number and location of all distillation regions and boundaries in the system.
- The feasible splits that can be achieved for a specified feed.

- The reflux ratio, number of theoretical stages and feed stage location for each feasible split.
- All feasible sequences that can separate a given feed into pure components and/or azeotropes.

3.2 Calculation Procedure

Column Sequencing generates feasible splits for a specified feed. Non-pure products of the first simple distillation columns are treated as feeds to a set of secondary distillation columns for which the feasibility split calculations are performed again. This calculation is continued until either all products are pure components, azeotropes, or reside on a distillation boundary. The figure below shows the general calculation algorithm to generate a sequence of distillation columns for isobaric conditions (i.e., all distillation columns will operate at the same pressure specified by the user).

Figure 3.1



For more information about the Design level, refer to **Section 3.5 - Design Level** from the **Azeotropic Separation** manual.

DISTIL determines a set of solutions to the problem of separating the feed mixture into its pure components or azeotropes. These process configurations/designs are displayed at the Design level of the Column Sequencing view.

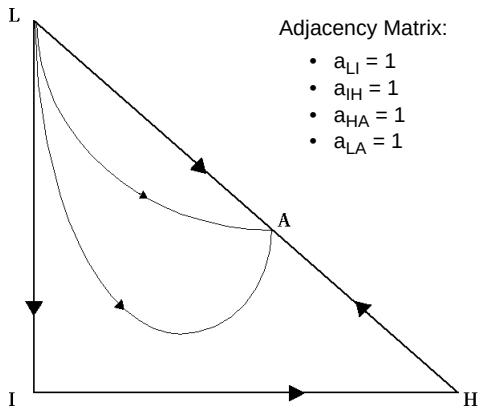
3.2.1 Adjacency Matrix

Adjacency matrix is a square matrix, which rows and columns correspond to pure components and azeotropes in the system. In order to construct the Adjacency matrix for a multi-component system, you must identify all "n" singular points (pure components and azeotropes) in the system and find out all the elements of the $n \times n$ matrix. Singular points are arranged in order of increasing boiling temperature. The elements of the adjacency matrix are either 0 or 1.

$$A = [a_{ij}] \qquad i, j = 1, ..., n \tag{3.1}$$

The element $a_{ij} = 1$, if there exists a residue curve that starts at singular point i and ends in singular point j. Element $a_{ij} = 0$ if there is no such residue curve. All elements on diagonal of the matrix are set to zero.

Figure 3.2



	L	I	H	A
L	0	1	0	1
I	0	0	1	0
H	0	0	0	1
A	0	0	0	0

The figure above displays a Residue Curve Map for a three component system with a maximum boiling azeotrope. **L** is the light component (lowest boiling temperature) of the system, while **H** is the heavy one (highest boiling temperature) and **I** is the intermediate boiling temperature component. **A** is the azeotrope. In this example, elements a_{LI}, a_{IH}, a_{IA} and a_{LA} are equal to one, while all others are zero.

The Adjacency matrix is an alternative representation of a Residue Curve Map with the advantage that it is not restricted to 3-dimensional

space. An unstable node is indicated by a column composed entirely of zeroes. The column (singular point *j*) is unstable since no other singular point can be connected to it. A stable node is indicated by a row composed entirely of zeroes. The row (singular point i) is stable since it cannot be connected to any other singular point.

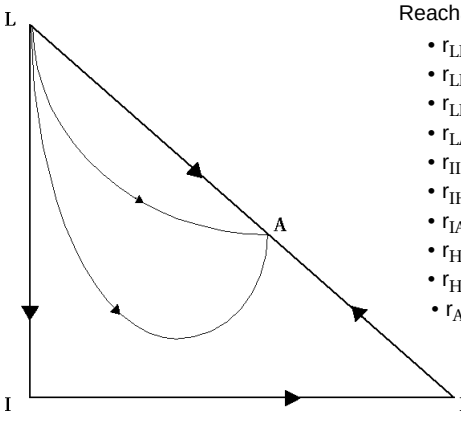
3.2.2 Reachability Matrix

Like the Adjacency matrix, the Reachability matrix is a square $n \times n$ matrix, where n is the number of singular points, arranged in order of increasing boiling temperature. The elements of the Reachability matrix are either 0 or 1.

$$R = [r_{ij}] \qquad i, j = 1, ..., n \tag{3.2}$$

The element $r_{ij} = 1$, if there is any path from a singular point *i* to *j*. Otherwise $r_{ij} = 0$. In other words, $r_{ij} = 1$, if singular point *j* can be reached from singular point *i*. The path from *i* to *j* can include a number of intermediate singular points. All elements on the diagonal of the matrix are equal to 1. The figure below displays the same RCM as in the previous figure.

Figure 3.3



Reachability Matrix:

- $r_{LL} = 1$
- $r_{LI} = 1$
- $r_{LH} = 1$
- $r_{LA} = 1$
- $r_{II} = 1$
- $r_{IH} = 1$
- $r_{IA} = 1$
- $r_{HH} = 1$
- $r_{HA} = 1$
- $r_{AA} = 1$

	L	I	H	A
L	1	1	1	1
I	0	1	1	1
H	0	0	1	1
A	0	0	0	1

It is possible for a residue curve to join all singular points in this particular RCM. From the figure above, all singular points can be reached from the singular point, *L*. It can also be observed that singular points *H* and *A* can be reached from singular point *I*.

The relationship between the Adjacency and Reachability matrices is as follows:

$$R = Boolean[A + I]^{n-1} \tag{3.3}$$

where: n = *the number of singular points*

I = *the Identity Matrix*

3.2.3 Distillation Regions and Boundaries

A distillation region is a collection of all residue curves which start at the same unstable node and end at the same stable node. Distillation boundaries separate distillation regions and usually cannot be crossed by a simple distillation. The distillation boundary is then a dividing line between families of residue curves for a 3-component system, and a dividing surface for a 4-component system. A distillation region is characterized by its stable and unstable nodes. Both products from a distillation column must be in the same distillation region for the design to be feasible.

The reachability matrix can be used to calculate the number of distillation regions in the system. The general procedure in determining the number of distillation regions is as follows:

1. Identify the stable singular point, *i*, and the unstable singular point, *j*, in the system using the adjacency matrix.
2. The number of regions is equal to the number of unstable-stable node pairs for which the element r_{ij} is 1.

3.2.4 Split Generator

The ability to predict a feasible top and bottom product composition is of immense value to the user.

DISTIL produces three different types of splits, a direct split, an indirect split, and an intermediate split.

- In the direct split, the highest pure component (or azeotrope) is removed as a top product. The bottom product lies on a distillation boundary or the composition boundary.
- Similarly, in an indirect split the heaviest pure component (or azeotrope) in the distillation region, is separated as a bottom product.

In theory, there is an infinite number of intermediate splits between the direct and indirect splits. DISTIL only produces those intermediate splits that produce complete separation of one component.

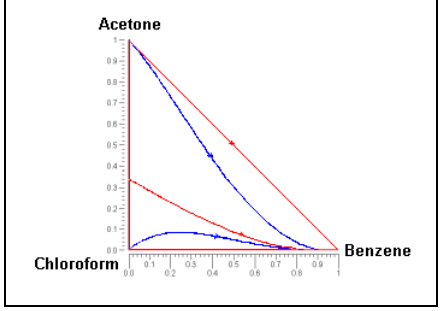
Each of the splits generated could be realized in practice using simple distillation columns. DISTIL predicts the minimum and actual reflux ratio needed to achieve this separation. Furthermore, it predicts the number of theoretical stages required to achieve the separation.

The following sections describe the procedure DISTIL used to locate the possible splits.

Establish Region Boundaries

First DISTIL establish the region boundaries of the mixture at the specified pressure.

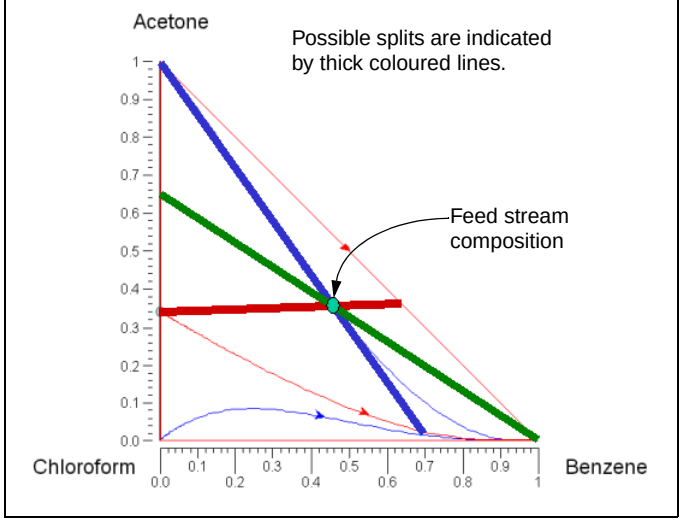
Figure 3.4



Location of Feed Stream

Second, DISTIL considers the location of the feed stream composition in a Component Space plot. From the plot DISTIL can locate multiple possible stream splits.

Figure 3.5



Check for Feasible Splits

Third, DISTIL selects the feasible splits out of all the possible splits by checking that the split meets two conditions:

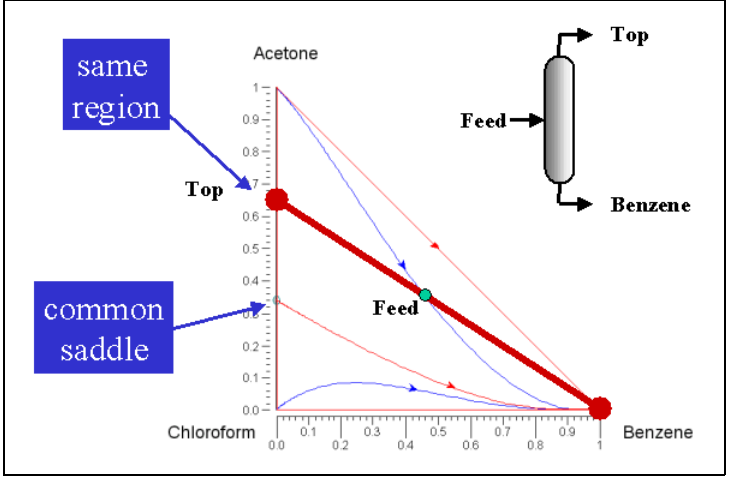
- Both products generated by the split is in the same region.
- Both products share a **common saddle**.

To illustrate how DISTIL selects the feasible splits the following three splits will be considered:

- Benzene as the bottom pure product.
- Acetone as the top pure product.
- Acetone-Chloroform azeotrope as the top pure product.

When benzene is the bottom product of the simple column split the following **feasible** split occurs.

Figure 3.6

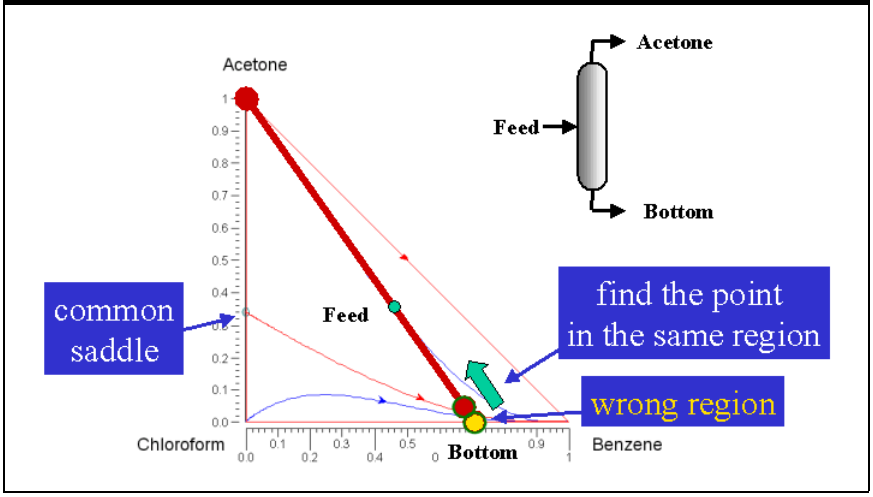


From **Figure 3.6**:

- The two product streams are in the same region.
- The composition point of the product streams both converged to a common saddle point.

When acetone is the top product of the simple column split the following **feasible** split occurs.

Figure 3.7



From **Figure 3.7**:

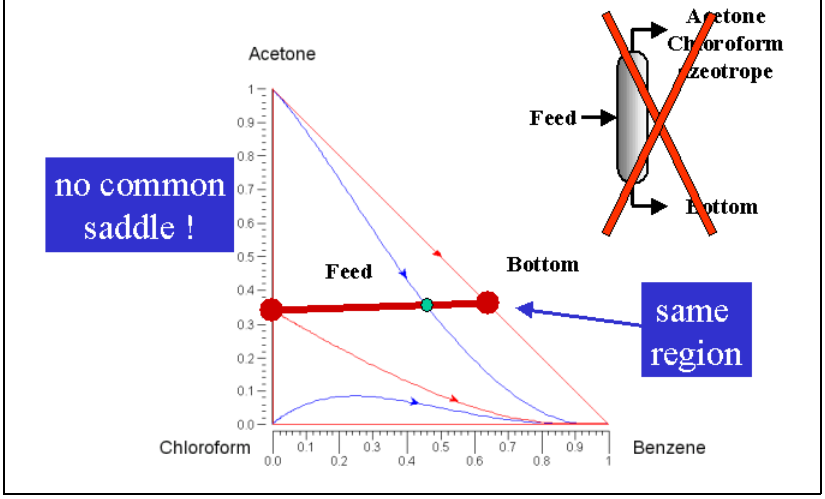
- The two product streams are in the same region.
  Notice the bottom product stream will still contain a little bit of acetone, because the product stream must remain in the same region.
- The composition point of the product streams both converged to a common saddle point.

When the acetone-chloroform azeotrope is the top product of the simple column split the following **infeasible** split occurs.

From **Figure 3.8**:

- The two product streams are in the same region.
- Unfortunately, the composition point of the product streams do not have a common saddle point.

Figure 3.8



Generate Column Design

Based on the information from the feasible splits, DISTIL will generate a feasible column design. The design of individual columns is performed using shortcut or more detailed geometric methods. Refer to **Chapter 4 - Azeotropic Distillation - Design Methods** for more information.

3.3 Sequence Evaluation

3.3.1 Assumptions

The following assumptions are made while performing the Column Sequencing calculation:

- All feasible sequences are generated using simple columns (each column has only two products, distillate and bottoms).
- Only primary recycles of the first and second kind are calculated. See Wasylkiewicz et. al. (2001)[165] for details.
- The default key tolerance for the product purity is 10^{-4}. This value can be changed by the user, and is in molar fractions.
- The default non-key tolerance represents the amount of small impurities of non-key components in the product. The non-key tolerance value is used to calculate minimum reflux, and the default value is $10^{-16.}$ This value can be changed by the user, and is in molar fractions.

3.3.2 Column Design

Each column of the sequence can be designed to estimate reflux, stages, etc.

DISTIL provides the user with an option to design each individual distillation column. For each column, the operating reflux, the number of stages and the feed stage location could be computed using Fenske-Underwood based shortcut techniques or using relatively more sophisticated geometric techniques.

The theory and assumptions of Fenske-Underwood based techniques is discussed in **Section 5.2 - Simple Column Design**.

The theory and assumptions behind the more sophisticated geometric methods for design of columns is discussed in **Section 4.4.2 - Geometric Method**.

3.3.3 Sizing and Costing

The theory and assumptions made in sizing and costing of each individual design can be found in **Chapter 9 - Size & Cost Assumptions**.

Having estimated the basic design parameters of each individual distillation column. DISTIL uses this information to perform shortcut sizing and costing. The sizing and costing information is used to predict an overall capital and operating costs for each individual design. So you can make a comparison of cost on all the designs generated.

3.4 Examples

Only primary recycles are considered in designing a separation sequence. However, you can also use DISTIL to find secondary recycles. The process is explained in **Chapter 8 - Use of Recycles** from the **Tutorial** manual.

3.4.1 Non-Isobaric Sequences (Pressure Swing)

The algorithm for automatic generation of feasible distillation column sequences for separation of multi-component mixtures at constant pressure (Rooks et. al., 1998[127]) has been extended to allow various pressures in individual distillation columns. It is based on rigorous feasibility test and split generation method for any number of components at a few selected pressures.

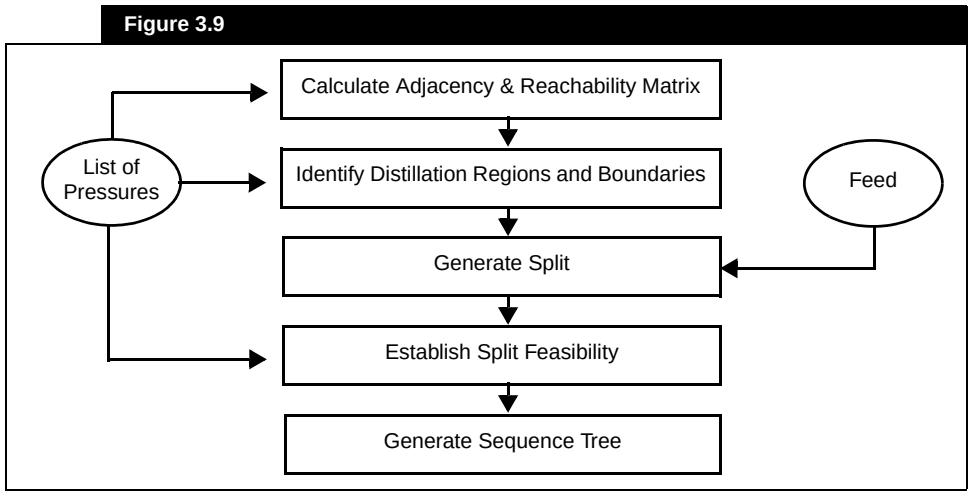
By varying the pressure we can identify opportunities for pressure swing distillation and heat integration between columns in the sequence. Pressure sensitivity analysis of azeotropes provides the dependence of their composition and temperature vs. pressure and can be very useful information for design of azeotropic distillation sequences.

By increasing or decreasing operating pressures in individual columns we can move distillation boundaries in the composition space or even make azeotropes to appear or disappear. This can have a tremendous effect on the topology of the residue curve map and the feasibility of distillation sequences.

In our pressure sensitivity analysis method, Wasylkiewicz et. al. (2000b)[168], we use bifurcation theory together with an arc length continuation method to find all bifurcation pressures, at which azeotropes appear or disappear, in a specified pressure limit.

The figure below shows the general calculation algorithm to generate a column sequence for non-isobaric conditions.

Figure 3.9



Recycle Streams and Non-Isobaric Sequences

DISTIL will detect when a stream can be recycled during generation of distillation sequence. One of the two following conditions have to be met for the recycle to be calculated:

- **Primary Recycle of the First Kind**. The composition of a product stream from the last added separator is equal to the composition of a feed stream already present in the partially synthesized sequence (Wasylkiewicz and Castillo, 2001[165]).
- **Primary Recycle of the Second Kind**. The composition of a product stream from the last added separator is not equal to the composition of the existing unit feed, although if added to the unit as a second feed will only change flow rates, but not compositions of the products (Wasylkiewicz and Castillo, 2001[165]).

Recycle streams can reduce significantly the number of columns required in a sequence.

The following outlines an example of a non-isobaric sequence including recycle streams generated by DISTIL.

Parameter	Value
Feed Flow	100 kmol/h
Feed Molar Composition	• Methanol: 0.33 • Methyl Acetate: 0.33 • Ethyl Acetate: 0.34
Pressures	100 kPa and 1000 kPa
Property Package	NRTL-Ideal

The results are outlined as follows:

Figure 3.10

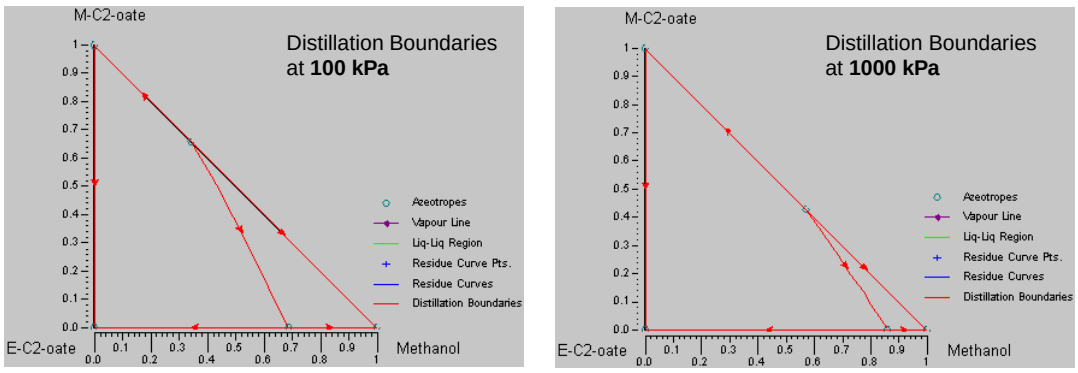
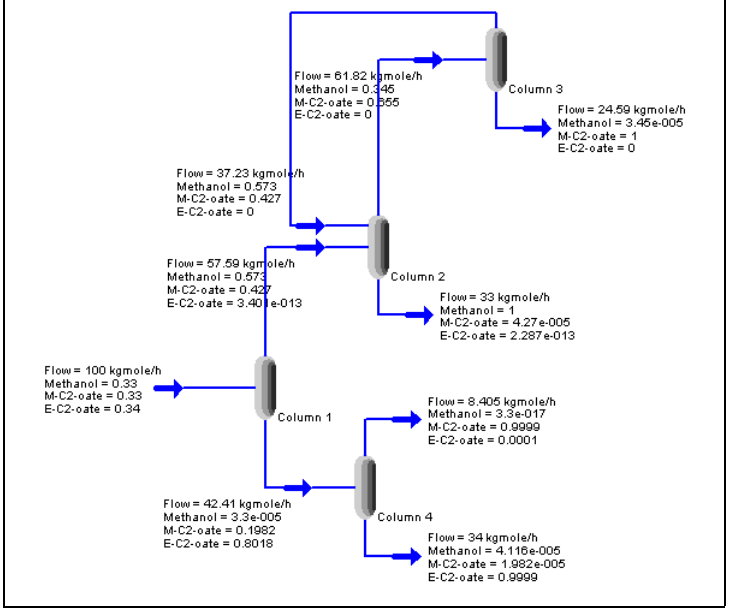


Figure 3.11



By allowing the splits to be performed at different pressures, azeotropes can be “broken” and boundaries can be crossed, since composition of azeotropes often depend strongly on the operating pressure. This algorithm enables DISTIL to automatically determine “pressure swing” schemes in any dimensional component space as well as in binary and ternary systems.

3.4.2 Designs with Decanter

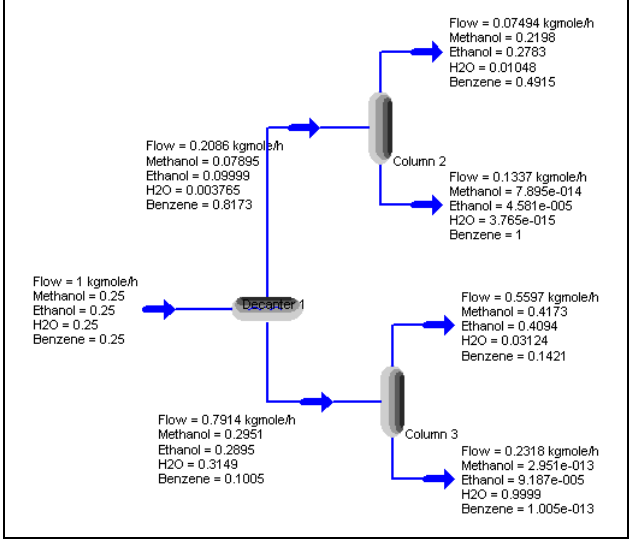
In the presence of heterogeneous liquids, it is useful to select the Decanter option. This will allow DISTIL to include decanters in the separation sequences. When this option is selected, DISTIL will attempt to find two liquid split for every stream in the sequence. For every two liquid split found, DISTIL will place a decanter in the separation sequence.

The following example briefly illustrates the benefits of using the decanter option when dealing with heterogeneous liquids.

Parameter	Result
Equimolar Feed without Decanter Option	3 Feasible Sequences found. All obtained pure water only
Equimolar Feed with Decanter Option	15 Feasible Sequences found. Some obtained pure methanol, water, and benzene.

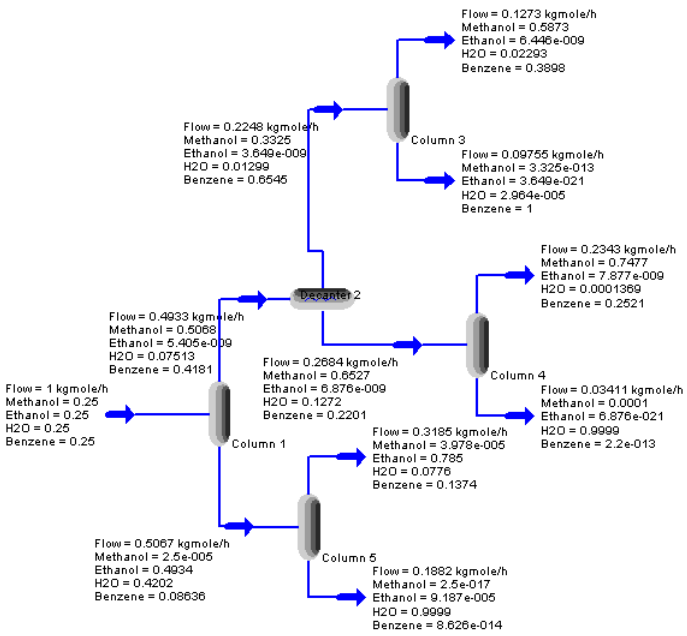
Listed below is one feasible sequence generated using the Decanter option.

Figure 3.12



Another feasible sequence is also listed below:

Figure 3.13



4 Azeotropic Distillation - Design Methods

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4.1 Introduction

The performance of the different columns in the sequence is evaluated using design methods. The minimum reflux and number of trays required for the separation are estimated using shortcut or geometric methods. Following sections describe various design methods employed by DISTIL.

4.2 Binary Distillation

DISTIL allows you to design *Binary Distillation* columns using the McCabe-Thiele technique. With the McCabe-Thiele technique, you can determine:

- the number of trays
- the minimum reflux ratio
- the range of feasible feed compositions
- and the optimal feed tray location

Most of the design information is conveniently located in the Column Design view, *Spec Entry* tab. As you provide the appropriate specifications on the *Spec Entry* tab, the McCabe-Thiele plot will be updated, allowing you to quickly set up the column parameters. Once you have designed an optimal column, you can move to other tabs to view additional results, such as the stage temperature and stage composition profiles.

4.3 Ternary Distillation

For more details on the BVDM, refer to the **Number of Theoretical Stages, feed stage location** section from **Section 4.4.2 - Geometric Method**.

The Ternary distillation uses Boundary Value design method (BVDM). The BVDM is an extension of McCabe-Thiele. It calculates the liquid composition profile from top product (rectifying profile) and bottom product (stripping profile) with a specified reflux/reboil ratio. If the two profiles intersect, then the column products are feasible. If the two profiles do not intersect, then the column products are not feasible.

4.3.1 Background

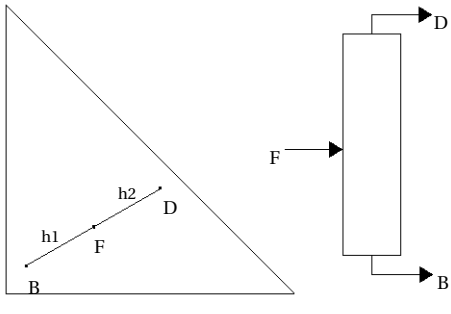
The following sections discuss the mass balance equations and assumptions for various Ternary Distillation columns.

Simple Column

A simple column schematic is shown in the right portion of the figure, illustrating the location of the feed and product streams.

The figure below illustrates the mass balance for a ternary distillation column with feed, distillate and bottoms streams.

Figure 4.1



The ternary composition diagram is shown in the left portion of the above figure. The points labelled *B*, *F*, and *D*, represents the composition of the Bottoms, Feed, and Distillate streams respectively. A mass balance of these streams requires that these three points line up in a straight line in the component space.

The flow rates can be determined from the lever rule (length of line segments *h1* and *h2)*.

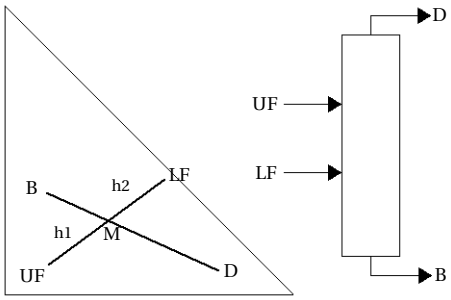
$$D_{FLOW} = F_{FLOW}\left(\frac{h1}{h1+h2}\right) \qquad B_{FLOW} = F_{FLOW}\left(\frac{h2}{h1+h2}\right) \tag{4.1}$$

Column with Two Feeds

A simple column schematic is shown in the right portion of the figure, illustrating the location of the feed and product streams.

The figure below illustrates the mass balance for a ternary distillation column with two feeds and two products (distillate and bottoms streams).

Figure 4.2



The overall feed point is located on the line connecting *point M*. The lever rule, which takes into account the relative flow rates, is used to determine the exact location.

The ternary composition diagram is shown in the left portion of the above figure. The points labelled *B, UF, LF,* and *D*, represent the composition of the Bottoms, Upper Feed, Lower Feed, and Distillate streams respectively. The overall feed point is labeled *M*. A mass balance of these streams requires that *B, M,* and *D* points line up in a straight line in the component space, like a simple column. The location of point *M* is also ruled by the following equation:

$$UF{:}LF = \frac{h_2}{h_1} \tag{4.2}$$

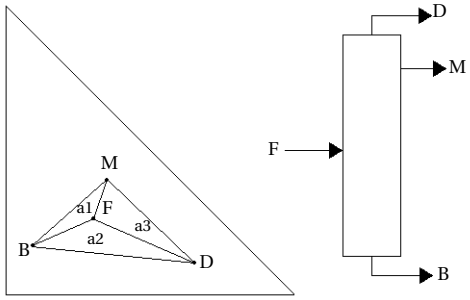
where: UF:LF = the flowrate ratio of the Upper Feed on the Lower Feed

Column with Sidestream

A column schematic is shown in the right portion of the figure, illustrating the location of the feed and product streams.

The figure below illustrates the mass balance for a ternary distillation column with one feed and three products (distillate, bottoms and side stream).

Figure 4.3



If there are two feeds, then the overall feed point is located on the line connecting them. The lever rule (which takes into account the relative flow rates) is used to determine the exact location.

The ternary composition diagram is shown in the left portion of the above figure. The points labelled *F, D, B,* and *M*, represents the composition of the Feed, Distillate, Bottoms, and Side streams respectively. It is required that the feed point *F* fall somewhere in the triangle formed by joining points *B*, *D,* and *M*.

It is possible to simultaneously obtain a near-pure bottoms and a near-pure distillate with this type of column configuration and a feed composition as shown.

The flow rates can be determined from the areas of $a1$, $a2$, and $a3$:

$$D_{FLOW} = F_{FLOW}\left(\frac{a1}{a1 + a2 + a3}\right)$$

$$M_{FLOW} = F_{FLOW}\left(\frac{a2}{a1 + a2 + a3}\right) \qquad (4.3)$$

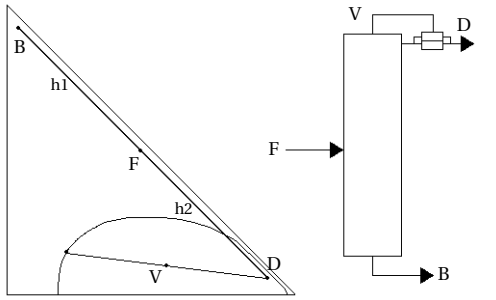
$$B_{FLOW} = F_{FLOW}\left(\frac{a3}{a1 + a2 + a3}\right)$$

Column with Decanter

The column configuration is shown in the right portion of the figure, illustrating the location of the feed and product streams, as well as the top vapour stream which enters the decanter, after being totally condensed.

The figure below illustrates the mass balance for a ternary distillation column with a decanter.

Figure 4.4



If there are two feeds, then the overall feed point is located on the line connecting them. The lever rule (which takes into account the relative flow rates) is used to determine the exact location.

The ternary composition diagram is shown in the left portion of the above figure. The points labelled *F, D, B,* and *V,* represents the composition of the Feed, Distillate, Bottoms, and Top Vapour streams respectively. It is required by the mass balance that points *B, F,* and *D* line up in a straight line in the component space.

Points *V* and *D* are both on the decanter line. The endpoints of the decanter line represent the two equilibrium liquid phases in the decanter. Point *D* will not be located on the endpoint, unless it is composed entirely of a single liquid phase from the decanter.

The flow rates can be determined from the lever rule.

$$D_{FLOW} = F_{FLOW}\left(\frac{h1}{h1+h2}\right) \qquad B_{FLOW} = F_{FLOW}\left(\frac{h2}{h1+h2}\right) \tag{4.4}$$

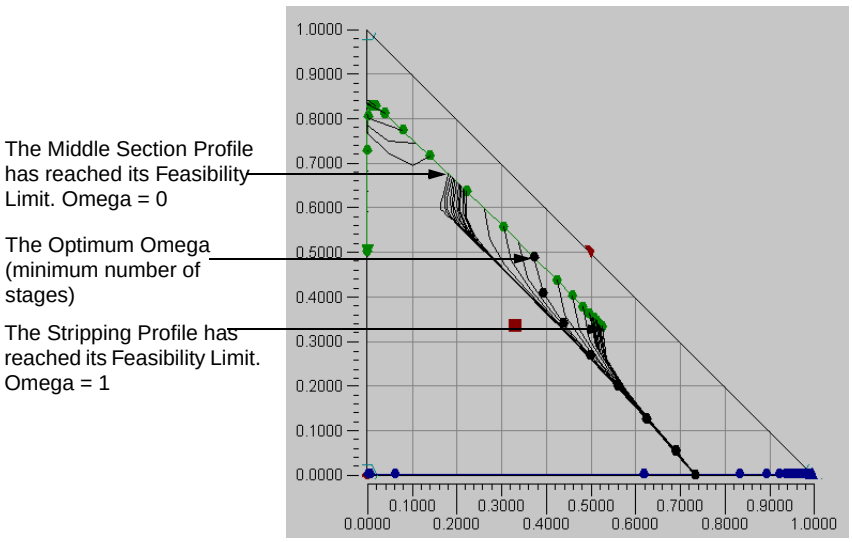
Omega Method

For some column configurations, DISTIL have an extra degree of freedom - feed stage location. To find the optimum value for feed stage location, DISTIL do one-parameter full search optimization, called *Omega Method* (Wasylkiewicz et. al., 2000a[167]).

For a binary distillation column, Omega is defined as a normalized distance between the stripping and rectifying pinch points. For a ternary distillation column, the Omega is calculated *only for two-feed distillation towers*, where it is defined as a normalized range of feasible second feed stage locations in the column.

The following is a *Component Space* plot with a range of middle profiles plotted. The middle section profiles are calculated upward (starting from stripping up to the intersection with rectifying profile). The range of Omega values encompass a range of feasible distillation double feed columns.

Figure 4.5



The optimum Omega value, which corresponds to a minimum number of stages, is calculated automatically for binary distillation and two-feed ternary distillation columns.

4.4 Multi-component Distillation

DISTIL offers two methods used to design columns for multi-component distillation: Shortcut and Geometric.

The following sections describe each method in detail.

4.4.1 Shortcut Method

This method is used to evaluate design parameters of a split, such as operating reflux, number of stages and feed stage location.

Underwood Method

A light key (*LK*) and a heavy key (*HK*) describe a split associated with each basic simple column. All the components lighter than *LK* come out with the distillate while heavier than *HK* components appear in the bottoms product. All the intermediate key (*IK*) components (i.e., components between the *LK* and *HK* in the ordered set) are either distributed optimally or the user fixes their distribution.

The first part of the Underwood equation (**Equation (4.5)**) is solved for each pair of components between the LK and HK to obtain Underwood roots θ_j.

$$\sum_{i \in I} \frac{x_i^f \cdot \alpha_i}{\alpha_i - \theta_j} = 1 - q \qquad \forall (j \in component\ pairs)$$
$$\alpha_{i+1} < \theta_j < \alpha_i \qquad \forall (i \in I) \tag{4.5}$$

where: α_{i+1}, α_i = *the relative volatilities*

q = *the quality of the feed stream*

x_i^f = *the molar feed composition*

All the values of Underwood roots θ_j are used in the second part of the Underwood equation (**Equation (4.6)**) to estimate the minimum reflux ratio.

$$\sum_{i \in I} \frac{x_i^d \cdot \alpha_i}{\alpha_i - \theta_j} = R^{MIN} + 1 \qquad \forall (j \in component\ pairs) \qquad (4.6)$$

where: x_i^d = *the molar distillate composition*

R^{MIN} = *the minimum reflux for the separation*

If you want to find the optimal distribution of *IK*s, then the **Equation (4.6)** is used with the mass balance equations simultaneously to yield x_i^d, distillate flowrate (*d*) and R^{MIN}. If the user fixes the distribution of IKs then the value of R^{MIN} for each Underwood root is estimated using **Equation (4.6)** and the controlling reflux (i.e., highest value of R^{MIN}) is calculated. The mass balance equations are then used to calculate the composition of the bottoms product x_i^b, bottoms flowrate (*b*) and the vapour liquid traffic.

Triantafyllou and Smith (1992)[152] and Shah (1999)[134] discuss the extension of this method for the Liquid side-draw column and the Vapour side-draw column.

Winn Model

Winn's method calculates the minimum number of stages (i.e., number of stages required at the total reflux) required for a desired separation. It is an extension of the Fenske method (Kister, 1992[71]) that accounts for the changes in the temperature of the column by introducing additional parameters β and γ. The following set of equations represents this model:

$$N^{MIN} = \frac{\ln[(x^d_{LK}/x^d_{HK}) \cdot (x^b_{HK}/x^b_{LK})]}{LN[\beta_{LK,HK}]} \tag{4.7}$$

$$\beta_{LK,HK} = \frac{K_{LK}}{[K_{HK}]^{\gamma}} \tag{4.8}$$

where: N^{MIN} = *the minimum number of stages*

β,γ = *the constants at the fixed pressure that are evaluated from the K-values of LK and HK at the top and bottom temperatures. They are related to each other by* ***Equation (4.8)****.*

Molokanov Equation

The actual number of theoretical stages required for the desired separation, when the column is operated at a specified *RF* (= R/R^{MIN} ratio), are calculated using the Molokanov equation (**Equation (4.9)**). The feed tray location is estimated using Kirkbride's correlation (**Equation (4.10)**). Expressions of this shortcut model are presented below.

$$\frac{NT - N^{MIN}}{NT + 1} = 1 - \exp\left(\frac{1 + 54.4 \cdot \aleph}{11 + 117.2 \cdot \aleph} \cdot \frac{\aleph - 1}{\aleph^{0.5}}\right) \tag{4.9}$$

where:

$$\aleph = \frac{RF - 1}{RF + 1/R^{MIN}} \tag{4.10}$$

$$\frac{NT^{above\ feed}}{NT - NT^{above\ feed}} = \left[\frac{x_{HK}^{f}}{x_{LK}^{f}} \cdot \left(\frac{x_{LK}^{b}}{x_{HK}^{d}}\right)^{2} \cdot \frac{b}{d}\right]^{0.206}$$

4.4.2 Geometric Method

If the feasible column calculation is not limited to direct/indirect splits when the Geometric method is selected, a warning view will appear.

Click the **OK** button in the warning view, and DISTIL automatically activates the option to limit the feasible columns to direct/indirect splits only.

The Geometric method is like the Shortcut method, in that it too is used to evaluate design parameters of a split. However, the Geometric method calculation is available for direct/indirect splits only.

Minimum Reflux

Minimum reflux calculations are calculated for a given feed and product specifications using the rectification body method presented by Bausa et. al. (1998)[13].

The minimum reflux calculations using the ROM have the following steps:

1. Determine the pinch points for a given reflux (or reboil) ratio, and for a singular point, as a distillate (or bottom) product. The distillate (or bottom) composition that could be reached, if an infinite number of stages are provided, is the pinch point composition.

   Pinch points are determined by solving the following equations for the rectification such as:

Equations (4.11) and **(4.12)** have multiple solutions and each solution is determined in DISTIL using continuation techniques.

$$y^{*}(x_p) - \frac{L_p}{L_p + D} \cdot x_p = \frac{D}{L_p + D} \cdot x_D \tag{4.11}$$

$$h_p^{v} - \frac{L_p}{L_p + D} \cdot h_p^{L} = \frac{D}{L_p + D} \cdot h_D - \frac{Q_D}{L_p + Q_D} \tag{4.12}$$

2. Generate a pinch point path. A pinch point path is a collection of product composition and pinch points with an increasing number of stable eigenvectors.
3. A thermodynamic consistency check is performed on each path.
4. The generated paths can now be used to approximate the manifold of column profile. A manifold can be created for rectification body and another manifold for stripping body.
5. DISTIL then check all numbers of both sets for intersection against each other. The value of reflux (or reboil) ration at which the manifolds just intersect is the value of minimum reflux.

Number of Theoretical Stages, feed stage location

See **Section 4.3 - Ternary Distillation** for more information.

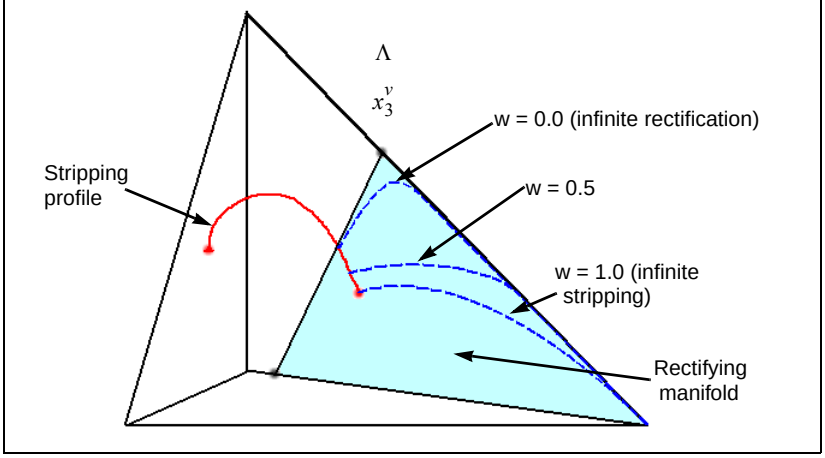
DISTIL provides a Boundary Value Design Method for designing columns with three components. For mixtures with four or more components, the boundary value method cannot be made to work in a satisfactory way.

The procedure used for calculation of number of stages was first developed by Julka and Doherty (1993)[67]. Here we summarize the steps involved:

1. Given the feed composition (x_f), feed quality (q), and column pressure (P), specify targets for distillate and bottom composition.
2. Calculate minimum reflux ratio using the procedure described before. Set the operating reflux, r = (1.2 - 1.5).
3. For a direct split, calculate the rectifying manifold using pinch points (as described in the previous section). Calculate the stripping profile from the specified product composition and the reboil ratio calculated above using mass and energy balance equation.
4. For a feasible split, the stripping profile will intersect the rectifying manifold. There are several combinations of theoretical stages in stripping and rectifying section that will satisfy the top and bottom product compositions.

DISTIL use the concept of displacement fraction (w)(Julka and Doherty, 1993[67]) to determine the number of stages. See the figure below:

Figure 4.6



4.4.3 Comparison between Shortcut and Geometric

The choice between the use of shortcut and geometric method is the classic tradeoff between speed and accuracy.

- Geometric methods are clearly more accurate and would work very well for highly non-ideal and azeotropic systems.
- Shortcut methods are limited in applicability to systems with near constant relative volatility. However, computation of design parameters using shortcut techniques is very fast.

Both techniques are limited in applicability to homogenous system for the current version of DISTIL. The applicability of both methods is limited to simple feed systems.

5 Non-Azeotropic Distillation

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5.1 Introduction

The aim of this chapter is to study the performance of various design options for the non-azeotropic system. The focus is on evaluating the performance (with minimum process information) quickly for the relative comparison of all options.

The first section describes performance models of simple columns. The next section discusses incentives, challenges, and modeling framework of the complex column configurations (that include dividing wall column, side-stripper arrangement, prefractionator design, etc.). The last section describes how rigorous optimization can be used to screen and scope large number of column sequences.

5.2 Simple Column Design

The Simple Column design feature/process provides a platform for the design and analysis of simple distillation column (i.e., column with one feed, one top product, one bottom product, one condenser, and one reboiler).

The Simple Column design separates a multi-component feed stream into two user defined products. The product is defined by a light and heavy components of the split and their recoveries in the product.

Once the basic process information is provided, then various shortcut methods are employed to evaluate the column design performance. The details of the method are given in the following sections.

5.2.1 Performance Models

The primary objective of the shortcut models here is to obtain the estimates for the vapour-liquid traffic (i.e., reflux and reboil ratios) and the number of trays in each section of the column. The minimum reflux ratio for the specified separation is calculated using Underwood method (Underwood, 1948[156]), while the minimum number of theoretical stages are estimated using Winn's method (Kister, 1992[71]). The actual reflux and the number of stages are then determined by employing Molokanov's correlation (King, 1980[70]) for the specified R/R^{MIN} value.

Triantafyllou and Smith (1992)[152] and Shah (1999)[134] discuss the extension of this method for the Liquid side-draw column and the Vapour side-draw column.

For more information regarding the methods used in the Shortcut model, refer to **Section 4.4.1 - Shortcut Method**.

All these methods make following two assumptions:

- Constant molar overflow (CMO).
- Constant relative volatility (CRV).

These assumptions restrict their applicability to the zeotropic systems. The geometric mean of relative volatilities from different sections is obtained to estimate a more realistic and representative set of volatility values that can be used in shortcut methods. However, it is recommended to carefully study the variation in relative volatilities values in different sections.

5.2.2 Sizing and Costing Methods

For more information about the sizing and costing methods, refer to **Chapter 9 - Size & Cost Assumptions**.

The shortcut model described in the previous section provides the necessary information from the column configuration to calculate the size and cost of the column design. DISTIL uses the temperatures from the condenser and reboiler to select the appropriate utility streams (based on the Pinch principles described by Linnhoff, 1993[97]) for the column design.

5.2.3 Optimising Column Pressure

DISTIL can optimise the operating pressure of the column to minimize one of the following objective:

- Total Annualized Cost
- Operating Cost
- Capital Cost
- Total Vapour Load
- Total Reboiler Duty
- Total Shaft Work

In the calculation to optimise the pressure, the user provides the upper and lower bounds for the pressure range. DISTIL will divide the range into number of intervals based on the available hot/cold utilities.

If the interval length is greater than 50% of the total range, then it is divided into a specified number of zones for further evaluation. The performance of the column is evaluated at each interval and compared to determine the optimum pressure.

5.2.4 Column Retrofit Options

Contrary to design, in Retrofit mode, the column height (in other words the number of trays) and column diameter are fixed, and it is desired to change the operating reflux and operating pressure to match the fixed column hardware.

Adjusting Reflux Ratio to Match Trays

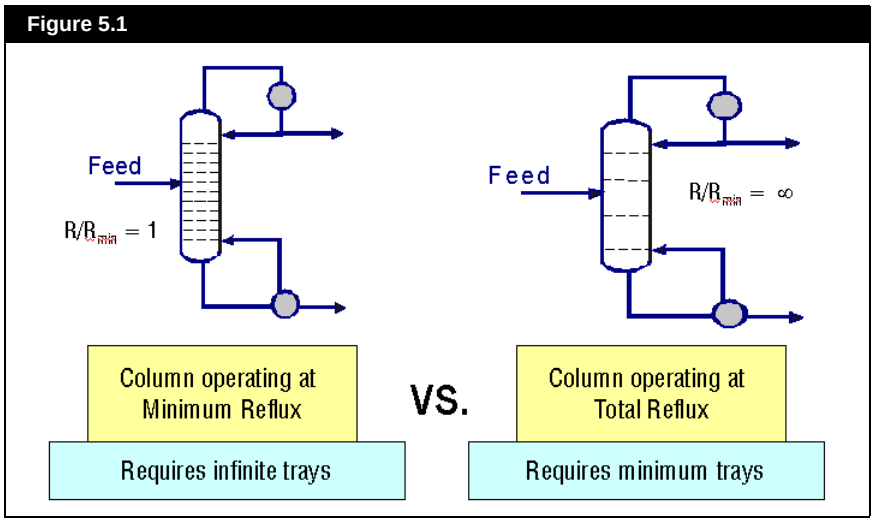
During the design mode, the operating reflux is obtained by multiplying minimum reflux value by a predefined number (R/Rmin) and then the number of trays are calculated.

To understand column operations, consider the following two extreme scenarios:

- A column with infinite number of trays, can achieve the desired separation with minimum reflux. This represents a “thermodynamic” limit or reversible column.
- A column with infinite reflux (or total reflux) can achieve desired separation with minimum number of trays. This represents an operating limit of the column.

Figure 5.1 displays the ideal column with minimum reflux ratio on the left side, while the ideal column with minimum number of trays is on the right side.

Figure 5.1

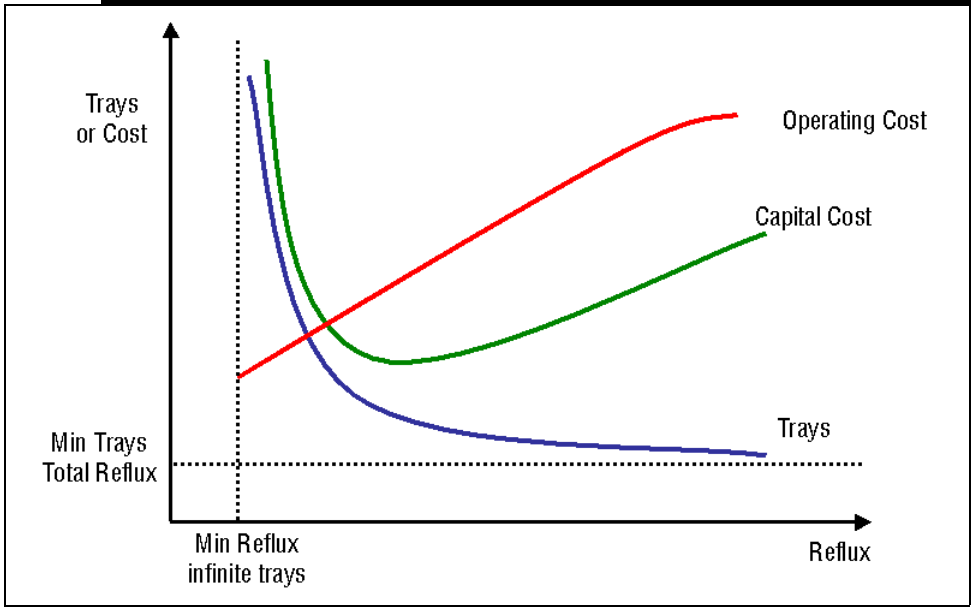


For more information about the Molokanov equation, refer to the **Molokanov Equation** section from **Section 4.4.1 - Shortcut Method**.

The understanding of the two extremes is used with Molokanov’s equation to predict the behaviour of real column at different reflux values above Rmin.

The figure below displays the relationship between the minimum reflux ratio and the number of trays/capital cost/operating cost:

Figure 5.2



As the column operating reflux increases above Rmin:

- The number of trays rapidly decreases. So capital cost decrease as well, but the operating cost increases due to increase in condenser and reboiler duties.
- The vapour traffic increases. So the column diameter increase as well. Hence the capital cost also increases slowly after a certain reflux value.

Thus in Retrofit mode, relationship between reflux and number of trays is evaluated.

Vary Operating Pressure to Match Diameter

There are two factors that affect/control the diameter of the trays in the column:

- **Vapour Density**. The density of the vapours flowing through the trays in the column.

  When the vapour density value is **small**, the vapour in the column requires more space/volume. So large tray diameter is required to increase the volume of the column and accommodate the large space.
  When the vapour density value is **large**, the vapour in the column requires less space/volume. So small tray diameter can be used to accommodate the small space, thus reducing the volume of the column.

- **Vapour/Liquid Traffic**. The ratio of the vapour/liquid flow rate through the trays in the column.

  When the vapour/liquid flow rate ratio value is **small** (less than 1), the amount of liquid in the column is more than the amount of vapour. So large tray diameter is required to hold the liquid at each stage/tray.
  When the vapour/liquid flow rate ratio value is **large** (more than 1), the amount of liquid in the column is less than the amount of vapour. So small tray diameter can be used to hold the liquid at each stage/tray.

The vapour density value can be modified by increasing/decreasing the operating pressure of the column.

- Increasing the operating pressure will increase the vapour density. The increase in operating pressure, however, will increase the difficulty in the separation process. When the difficulty of the separation process increases, more trays are required in the column to achieve the required/specified separation.
- Decreasing the operating pressure will decrease the vapour density.

The vapour/liquid flow rate ratio depends on the required/specified composition of the product streams.

- Increasing the number of light components in the top product will increase the vapour/liquid flow rate ratio. However, you may not achieve the required/specified separation.

- Decreasing the number of light components in the top product will decrease the vapour/liquid flow rate ratio. However, once again you may not achieve the required/specified separation.

5.3 Complex Column Configuration

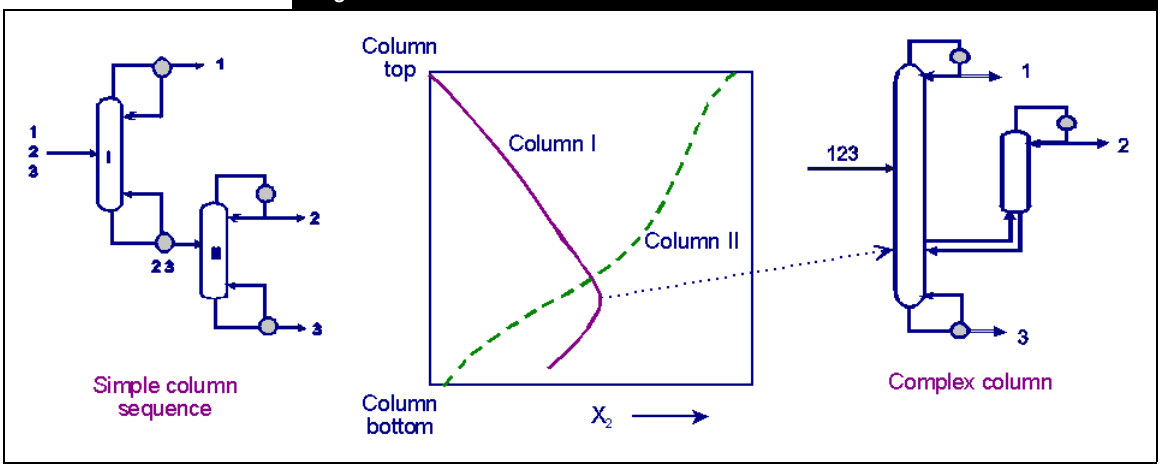
The tighter environmental regulations, higher energy costs, and growing competition have increased the drive for making distillation systems more efficient. Complex columns offer tremendous opportunity in improving efficiency of the distillation train.

There are several advantages to using complex column and several challenges in deciding which is the best configuration for your system.

5.3.1 Advantages of Complex Columns

The primary source of inefficiency in multi-component simple distillation is due to the irreversible mixing of non-identical streams. Simple columns are forced to sacrifice efficiency to achieve specified product specification in the multi-component systems. See the composition profile of component 2 in the figure below.

Figure 5.3

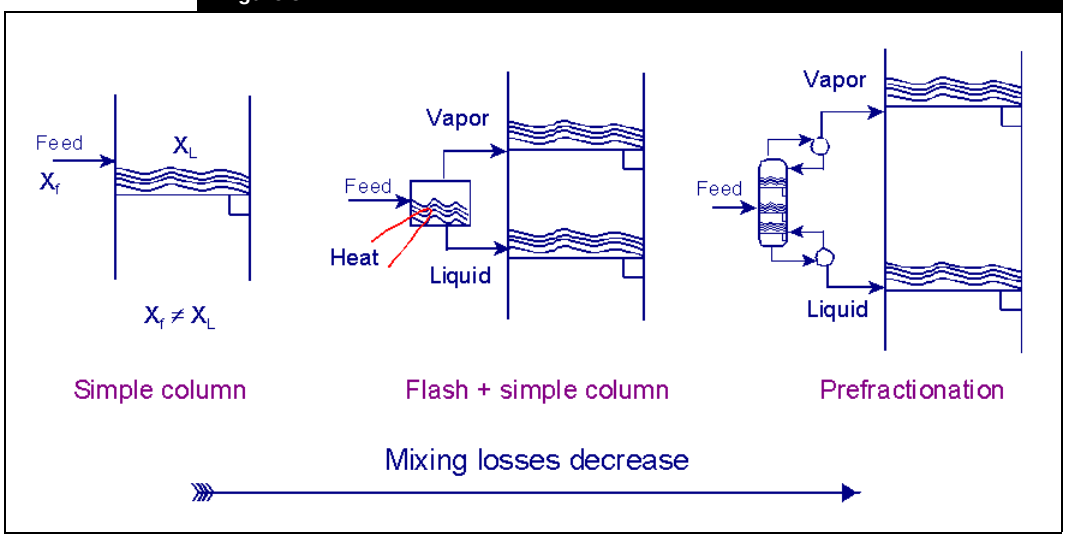


The figure above shows the concentration of the middle boiling components often reaches a maximum value on intermediate trays and

then decreases to satisfy overall mass balance. This *re-mixing* (or also called back-mixing) inherently affects the efficiency of separation. Another potential source of mixing is due to the differences in composition of the feed stream and the liquid composition on the feed tray (even after optimising feed tray location). Employing complex column configurations can minimize these mixing losses.

Complex columns offer a tremendous opportunity by reducing energy consumption and decreasing capital cost as well. They promote greater interaction between available vapour and liquid streams by introducing thermal coupling amongst different sections. They introduce additional sections (e.g., Side-rectifiers) to minimize re-mixing of middle boiling components (see **Figure 5.3**). They employ prefractionators to minimize feed tray mixing loss (see **Figure 5.4**).

Figure 5.4



These structural modifications in the distillation system improve energy efficiency that often results in energy savings (up to 30%). These columns require fewer column shells and heat exchangers (as condensers and reboilers) that decreases capital cost by up to 25%. Many researchers (Triantafyllou and Smith, 1992[152]; Fidkowski. and Krolikowski, 1986[41]) have reported up to 30% savings in energy and capital cost of the separation systems when appropriate complex column is used.

5.3.2 Challenges of Complex Columns

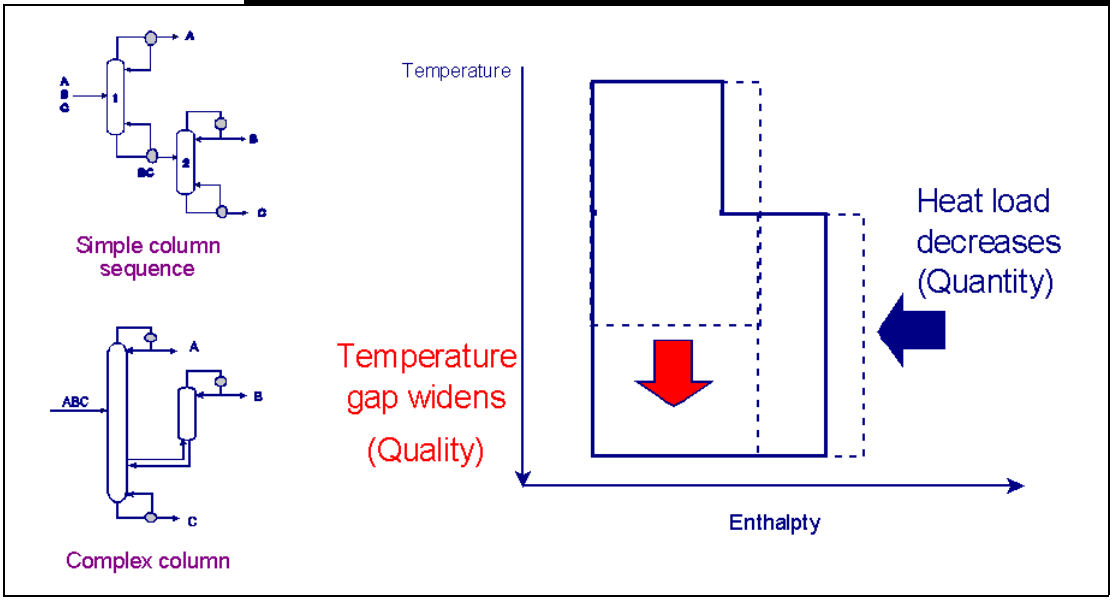
Complex columns introduce a large number of design options. Designers need to identify what type of complex column to use for the separation. For example, one can use side-stripper, side-rectifier, prefractionator, dividing wall column, or Petlyuk column to perform the same separation. Also one needs to decide where to use complex columns, whether to use them in the beginning of the sequence or towards the end of the sequence.

The thermal coupling in complex columns impose constraints on the operating pressures of the column sections. This creates a delicate balance between the ease of separation (relative volatility) and reflux requirements. For example, the direct sequence can operate two columns at two different and independent pressures, but when the complex columns are employed for the same separation the entire configuration has to operate at a single pressure to allow natural flow of vapour. In this scenario, one of the splits take place at non-optimum pressure and this results in higher reflux requirements. So, although the separation efficiency of the complex configuration increases, pressure constraints may have an adverse effect on column duties.

Pressure constraint also widens the temperature gap between the heating and the cooling loads. This may force the use of more expensive hot and cold utilities. So, the thermal coupling improves separation efficiency which in turn reduces column duties, but pressure constraint shifts that load to the extreme temperatures (see **Figure 5.5**). In other words, you encounter a complicated trade-off between the quality (temperature) and the quantity (heat load) of the energy. This energy trade-off is difficult to evaluate.

The figure below displays the energy trade-offs between a simple column sequence and a complex column.

Figure 5.5



Furthermore, the lack of comprehensive design and synthesis procedure poses difficulties in evaluation of large number of options and their complicated trade-offs. The concerns about control, operability and flexibility of the design add more roadblocks in the applications of the complex columns. The challenge here is to develop an integrated design framework to evaluate the performance of complex columns from its shortcut design to dynamic analysis.

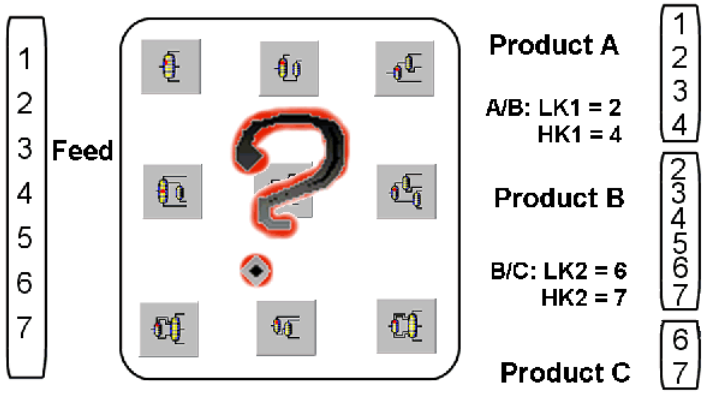
The complex column module in DISTIL provides a Life-Cycle-Solution^{TM} for the synthesis, design, and analysis of the complex columns to separate multi-component feed of zeotropic (i.e., non-azeotropic) system into the three specified products. It compares the performance of complex configurations like dividing-wall-column, Petlyuk column, partially coupled prefractionator arrangement, prefractionator arrangement, side-rectifier and side-stripper with simple column sequences, including distributed sequence. It provides a flexible and generic platform to visualize and analyse complicated trade-offs and improve synergy amongst different design stages by seamlessly integrating it with steady state and dynamic simulation in the HYSYS environment.

5.3.3 Specification of Three Product System

The specification of three product system separates a multi-component feed stream into three products by defining two splits and specifying two light (*LK1* and *LK2*) and two heavy splits (*HK1* and *HK2*).

The figure below illustrates the separation of seven-component feed stream into three products and describes all key definitions.

Figure 5.6



The selection of key components obey the following equation to ensure the feasibility of the separation using distillation in the zeotropic systems where component order does not change with operating conditions.

$$1 \le LK1 < HK1 \le LK2 < HK2 \le m \tag{5.1}$$

where: 1, *m = the component indices of the first and the last components after arranging them in the order of decreasing volatility.*

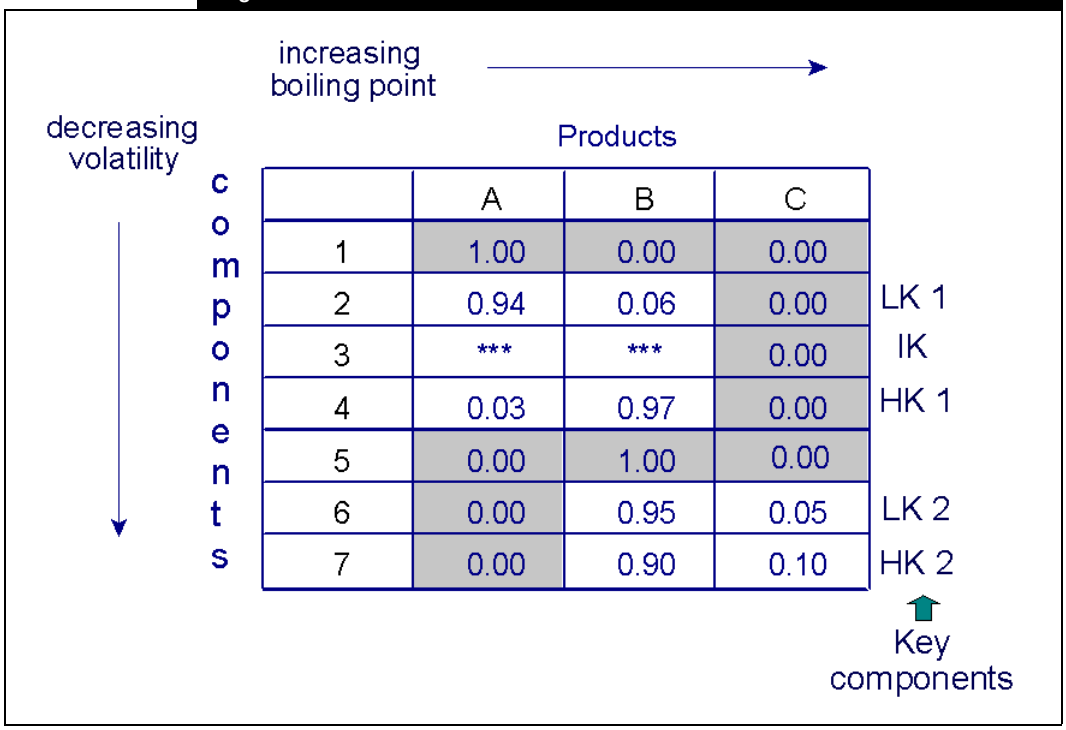
Unlike previous methods that used lumping or hypocomponents for each product, the multi-component nature of the products is addressed with the use of a recovery matrix. The matrix rows are the components (listed in the order of decreasing volatility) and the matrix columns are the products (whose normal boiling point increases from left to right). The matrix elements are fractional recoveries of the components in each product.

It is important to note that the light and heavy keys of the split need not be adjacent.

It is assumed that all the lighter than light key components appear only in the top product of the split while the heavier than heavy key components go exclusively with the bottom product. This allows DISTIL to fill the recovery matrix automatically once the light and heavy keys are selected. All the components between the two keys (also called intermediate key components) can be distributed in the top and the bottom products of the split. It is possible to either optimise the distribution of intermediate keys or specify it to any predefined value between 0 and 1. Depending on the option chosen by the user, calculation method will vary. The details of the calculation method are given in the next section. The detailed discussion about the recovery matrix is presented in Shah (1999)[134].

The figure below illustrates a recovery matrix of seven components {1,2, ...7} to be separated into three products A, B and C.

Figure 5.7



The recovery matrix also describes the light and heavy keys of the two splits. The first split has a nonadjacent light and heavy keys and the distribution of the intermediate key (i.e., component 3) is optimized (as

denoted by *** in the recovery matrix). The features of the separation scheme described by the recovery matrix products are apparently different from a scheme described by components. For example, the sharp separation between the products A and B (from the figure above) corresponds to a non-sharp separation between components 2 and 4 with the specified recoveries.

The important advantages of the recovery matrix representation are:

- Requires minimum information to specify the separation problem.
- Handles multicomponents nature of the products without lumping components.
- Specifications are independent of basis (like mole or mass or liquid volume).
- Ensures the feasibility of the separation in all zeotropic systems.

5.3.4 Complex Column Design Options

In this section, all the potential design options to separate three products from the single feed are discussed in more detail.

When the system requires a single feed stream be split into three product streams, there are some advantages in using certain complex columns. The advantages are based on the composition of the feed stream.

For example, if the product streams split ratios for the components relative volatilities both equal *2* and the feed stream contains:

- 0.40 mole fraction of product A (Top product stream)
- 0.20 mole fraction of product B (Middle product stream)
- 0.40 mole fraction of product C (Bottom product stream)

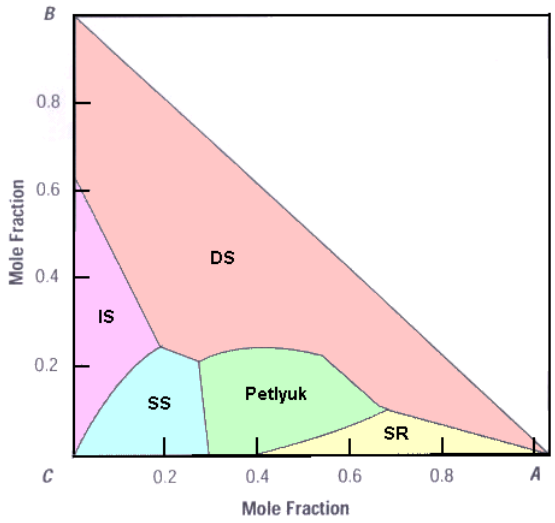
The Petlyuk column design is the most efficient design to use to separate the feed stream.

The decision for the optimum design is based on the optimality regions of different configurations on a composition space plot (from Agrawal & Fidkowski, 2002[2]).

The plot in the figure on the right and other similar plots are useful in gaining insights on the most efficient complex column configuration.

However, the plots are hard to use for evaluating the complicated tradeoffs related to the quality vs. quantity for energy in utilities or the effect of pressure constraints.

Figure 5.8



Optimality regions of different configurations on the composition space (for $\alpha_{A/B} = \alpha_{B/C} = 2$).

where:

α = *the split ratio between the product streams' relative volatilities*

DS = the direct sequence

IS = the indirect sequence

SR = the side rectifier

SS = the side stripper

A brief description of each complex column configuration and its advantages and limitations are discussed in the following sections.

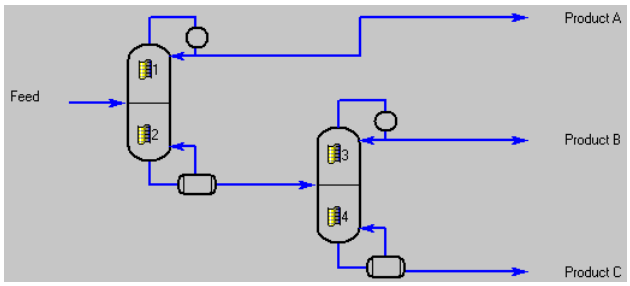
Simple Column Sequences

The sequence consists of two or more simple columns (i.e., a column with a single feed, two products, one condenser, and one reboiler) connected by a single stream. For three-product system, the following simple column sequences can be generated.

Direct Sequence

In the direct sequence, the first column separates the lightest product as the distillate and the rest is fed to the second column to perform the downstream separation as shown in the figure below:

Figure 5.9



The operating pressures of columns can be optimized independently to perform the first and the second splits respectively as they employ independent column shells and are connected by a liquid stream.

Optimal design when:

$\alpha_{B/C} < 1.5 < \alpha_{A/B}$

where:

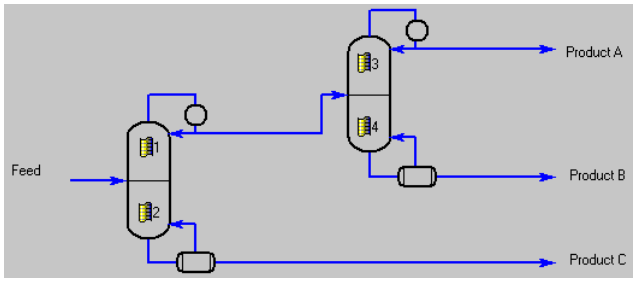
α = *the relative volatility*

The direct sequence is most promising when feed stream has a large quantity of product A and/or the separation involves difficult second split (i.e., B/C). It is often used to separate natural gas liquids into C3, C4, and C5+. It is the most widely accepted sequence of distillation columns due to its simplicity.

Indirect Sequence

Indirect sequence reverses the sequence of split by separating the heaviest product first. The distillate of the first column is fed to the second column to carry out the further separation as shown in the figure below:

Figure 5.10



The operating pressures of columns can be optimized independently as long as the first column uses a total condenser. However, this freedom is lost whenever the first column employs partial condenser. In that case, the second column is forced to operate at a lower pressure than the first column to ensure natural flow of vapour (without the use of a compressor).

Optimal design when:

$\alpha_{A/B} < 1.5 < \alpha_{B/C}$

where:

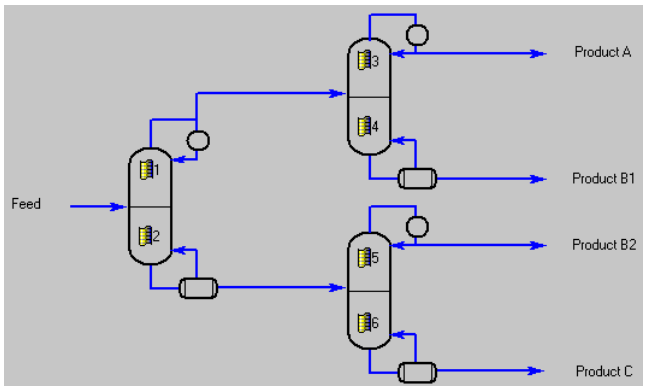
α = *the relative volatility*

The indirect sequence configuration is most promising when feed stream has a large quantity of product C and/or the separation involves a difficult first split (i.e., A/B).

Distributed Sequence

Unlike other simple sequences where each column produces at least one final product, this sequence employs distributed split to minimize mixing losses.

Figure 5.11



A distributed sequence uses a three-column sequence, where the first column separates product A completely from C and allows product B to distribute between the distillate and the bottoms to minimize the column reflux ratio. The distillate of the first column are fed to the second column to separate A from B while the third column is fed with the bottoms of the first column to separate B from C. The separation efficiency of the sequence is highest when a partial condenser is used on the first column (Fidkowski and Krolikowski, 1987[42]). However, it imposes a lower bound on the operating pressure of the second column. The operating pressures of the other columns can be optimized independently.

This sequence shifts part of the heating and cooling loads to the intermediate levels (on the reboiler and the condenser of the first column), hence it can use low quality (i.e., warmer cold utility or cooler hot utility) energy. However, it often requires higher capital investment (as it needs more column shells and heat exchangers).

Optimal design when:

$\alpha_{A/B} \sim \alpha_{B/C} < 1.5$

where:

α = *the relative volatility*

The distributed sequence configuration is most promising when feed stream has a large quantity of product B (i.e., mole fraction of B > 0.30) and/or both the splits are difficult. It is extremely useful in the sub-

ambient processes and while revamping distillation train to increase throughput.

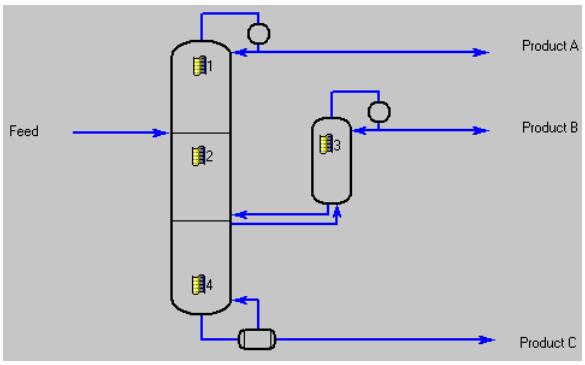
Thermally Coupled Arrangements

The thermally coupled arrangements are realized by setting up two-way vapour-liquid flow between different columns of the simple sequences. It often eliminates condenser and/or reboiler of the simple column while introducing vapour-liquid connection. By changing the sequence of splits and the level of thermal coupling, the following complex column configurations are generated. In this section, thermodynamically equivalent diagrams, advantages and limitations of those configurations are discussed.

Side-rectifier Arrangement

Side-rectifier arrangement consists of a thermally linked rectifier section with the main column as shown in the figure below:

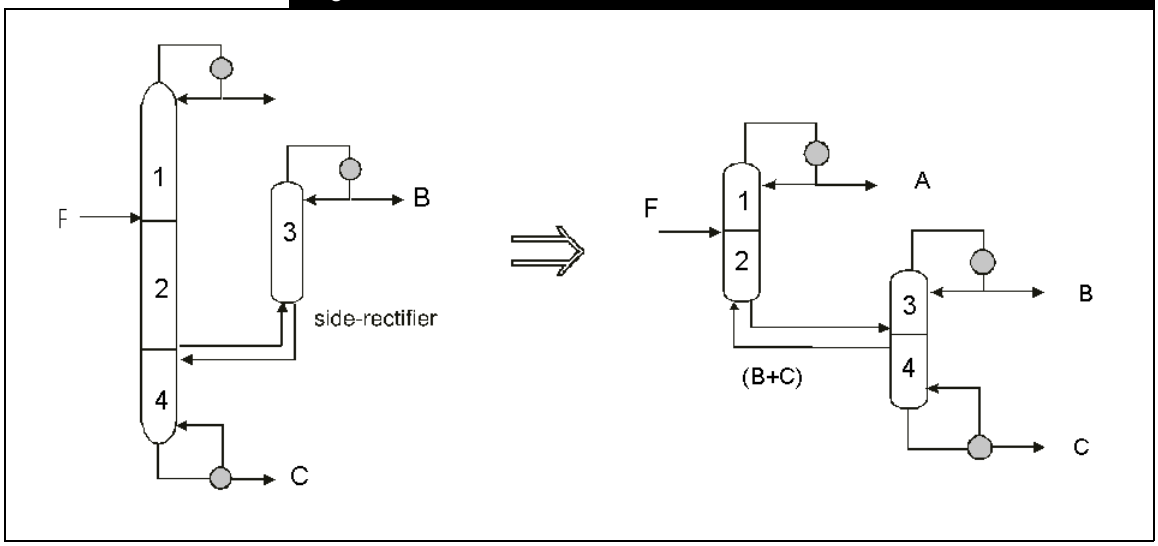
Figure 5.12



It produces all stripping vapour using only one reboiler but employs two condensers to provide rectifying liquid. The main column is forced to operate at the higher pressure than the side-rectifying section to allow natural flow of vapour. It achieves higher separation efficiency by imposing constraint on the operating pressure.

This arrangement can be decomposed into a thermally coupled direct sequence where the reboiler of the first column is eliminated by introducing two-way vapour-liquid connection as illustrated in the figure below:

Figure 5.13

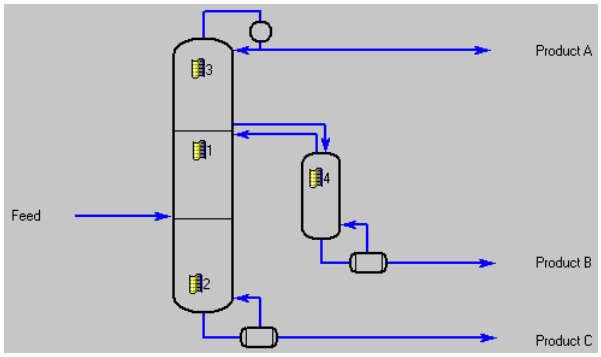


The side rectifier configuration is most promising when the feed stream contains high concentration of product A (i.e., mole fraction of A > 0.40). Some variations of this configuration is used to recover argon from air.

Side-stripper Arrangement

Side-stripper arrangement consists of a thermally linked stripping section with the main column as shown in the figure below:

Figure 5.14



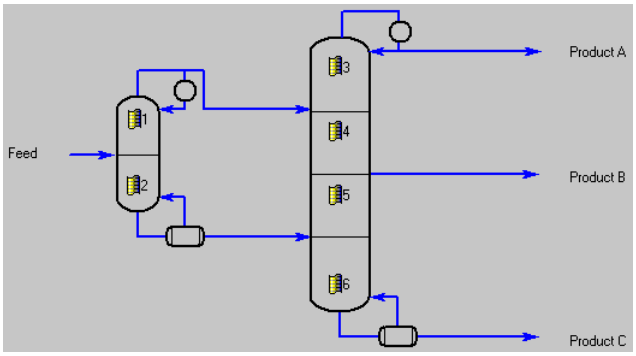
It produces all rectifying liquid using only one condenser but employs two reboilers to provide stripping vapour. The side-stripping section is forced to operate at the higher pressure than the main column to allow natural flow of vapour. It also achieves higher separation efficiency by imposing constraint on the operating pressure. This arrangement can be decomposed into a thermally coupled indirect sequence where the condenser of the first column is eliminated by introducing two-way vapour-liquid connection.

The side stripper configuration is most promising when the feed stream contains high concentration of product C (i.e., mole fraction of C > 0.50). This configuration is extensively used as a basic unit of a crude distillation tower.

Prefractionator Arrangement

Prefractionator arrangement employs two columns where the first column (also called prefractionator column) fractionates the feed (similar to the first column of the distributed sequence) and creates two feeds for the second column (also called main column). The main column features four sections and produces product A as the distillate, product B as the side-draw and the product C as the bottoms as shown in the figure below:

Figure 5.15



This arrangement is derived from the distributed sequence hence they display a number of similarities. The use of a partial condenser on the first column improves the separation efficiency of the configuration, however it imposes a lower bound on the operating pressure of the second column. The thermal coupling between the second and the third column of the distributed sequence results in the main column. It replaces the reboiler of the second column and the condenser of the third column with two-way vapour liquid connection.

Optimal design when:

$\alpha_{A/B} \sim \alpha_{B/C} < 1.5$

where:

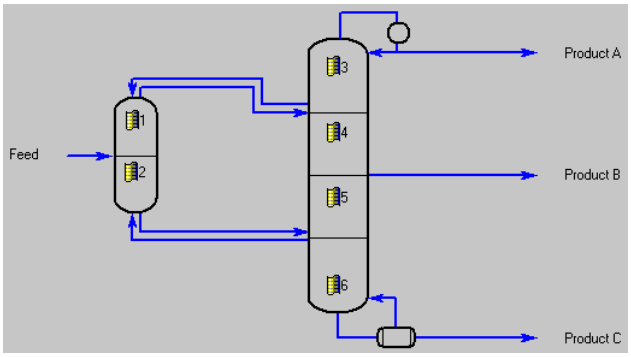
α = *the relative volatility*

The prefractionator configuration is most promising when the feed stream contains high concentration of product B (i.e., mole fraction of B > 0.30) and/or both the splits are difficult. In a styrene process, for example, a prefractionator is used to separate the styrene from the reactor effluent stream.

Petlyuk Column

This configuration introduces additional thermal links between the first (prefractionator) and the second (main) column of the prefractionator arrangement to improve efficiency. It replaces the condenser and the reboiler of the first column with thermal couplings as shown in the figure below:

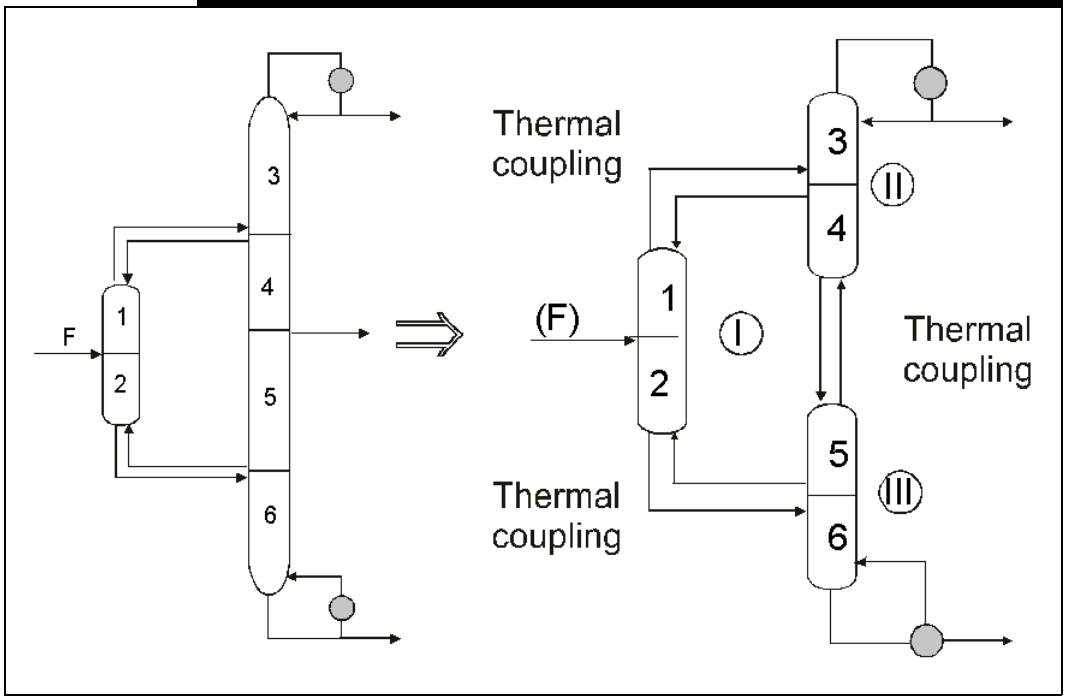
Figure 5.16



The thermodynamically equivalent arrangement of Petlyuk column is presented in **Figure 5.17**. This thermal integration minimizes separation losses and improves vapour-liquid interaction (i.e., higher effective rectifying or stripping ratios) in all sections of the columns. This arrangement requires the least amount of stripping vapour or rectifying liquid among all the options of the three-product system.

Petlyuk et al. (1965)[113], Fidkowski and Krolikowski (1987)[42] present the detailed analysis of this arrangement.

Figure 5.17

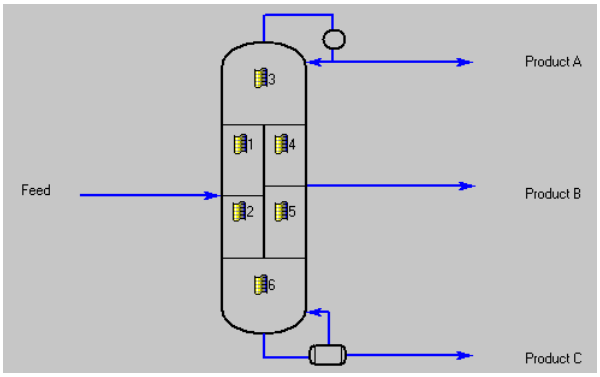


The two way vapour transfer between the two columns (i.e., vapour is fed to the main column at the top of the first column, while at the bottom of the first column, vapour is supplied by the main column) not only imposes strict pressure constraints, but also pose control and operability challenges.

Dividing Wall Column (DWC)

The dividing wall column is essentially Petlyuk column operating in a single column shell. It introduces a vertical partition (wall) inside the column shell to accommodate prefractionator in the same column shell. It splits the stripping vapour (from main reboiler) and the rectifying liquid (from the main condenser) on the two sides of the wall to perform effective separation.

Figure 5.18

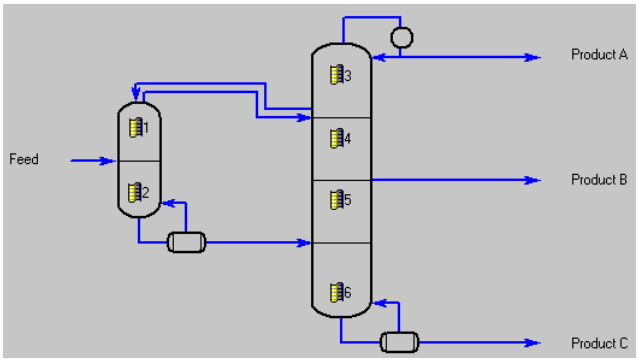


This allows a massive saving in the capital investment of the separation system and increases the separation efficiency at the same time. The only difference between the DWC and Petlyuk column is the heat transfer across the wall. A detailed discussion on the cases when the heat transfer across the wall is beneficial and when they have adverse effect is presented by Lestak et al. (1994)[84].

Partially Coupled Prefractionator

The partially coupled prefractionator configuration replaces the first column condenser of the prefractionator arrangement with a vapour-liquid connection but unlike Petlyuk column, retains the reboiler thus featuring an intermediate level of thermal coupling. (Agrawal and Fidkowski, 1999[1]) It uses two column shells and tries to maximize the benefits of thermal coupling without sacrificing the control characteristics.

Figure 5.19



By operating the first column at slightly higher pressure than the main column, the operability and controlability can be improved dramatically. The reboiler of the first column shifts a part of the heating load at the lower temperature, so this configuration can often employ a cheaper hot utility. All these issues make this configuration extremely attractive.

Optimal design when:

$\alpha_{A/B} < \alpha_{B/C} < 1.5$

where:

α = *the relative volatility*

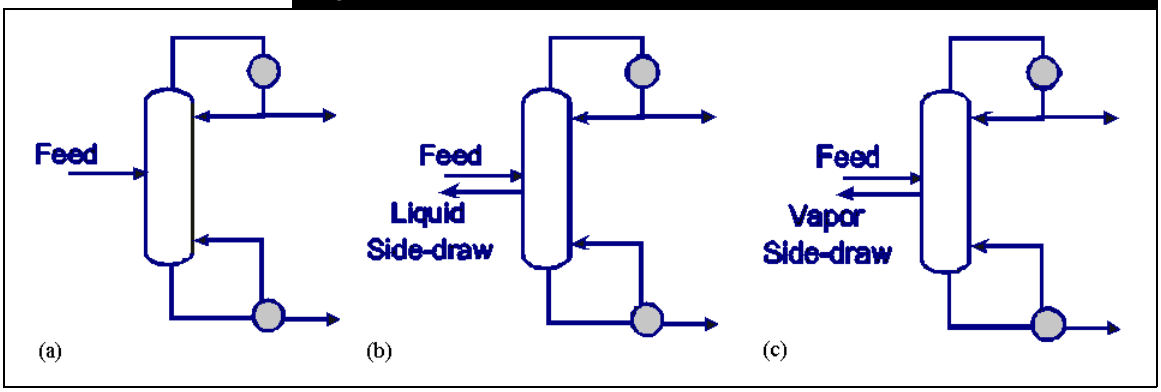
The partially coupled prefractionator configuration is most promising when the feed stream contains high concentration of product B (i.e., mole fraction of B > 0.30) and the first split is slightly more difficult than the second split.

5.3.5 Modeling of Complex Columns

Each complex column configuration is decomposed in the thermodynamically equivalent arrangement of the simple sequences. These thermally coupled sequences are further decomposed using different types of simple columns. Triantafyllou and Smith (1992)[152] have suggested following three basic simple columns to represent all thermal couplings:

- Simple column (**Figure 5.20** a): one feed, one distillate, and one bottoms product.
- Liquid side-draw column (**Figure 5.20** b): one saturated vapour feed, a saturated liquid side-draw from the feed tray, one distillate, and one bottoms product.
- Vapour side-draw column (**Figure 5.20** c): one saturated liquid feed, a saturated vapour side-draw from the feed tray, one distillate, and one bottoms product.

Figure 5.20



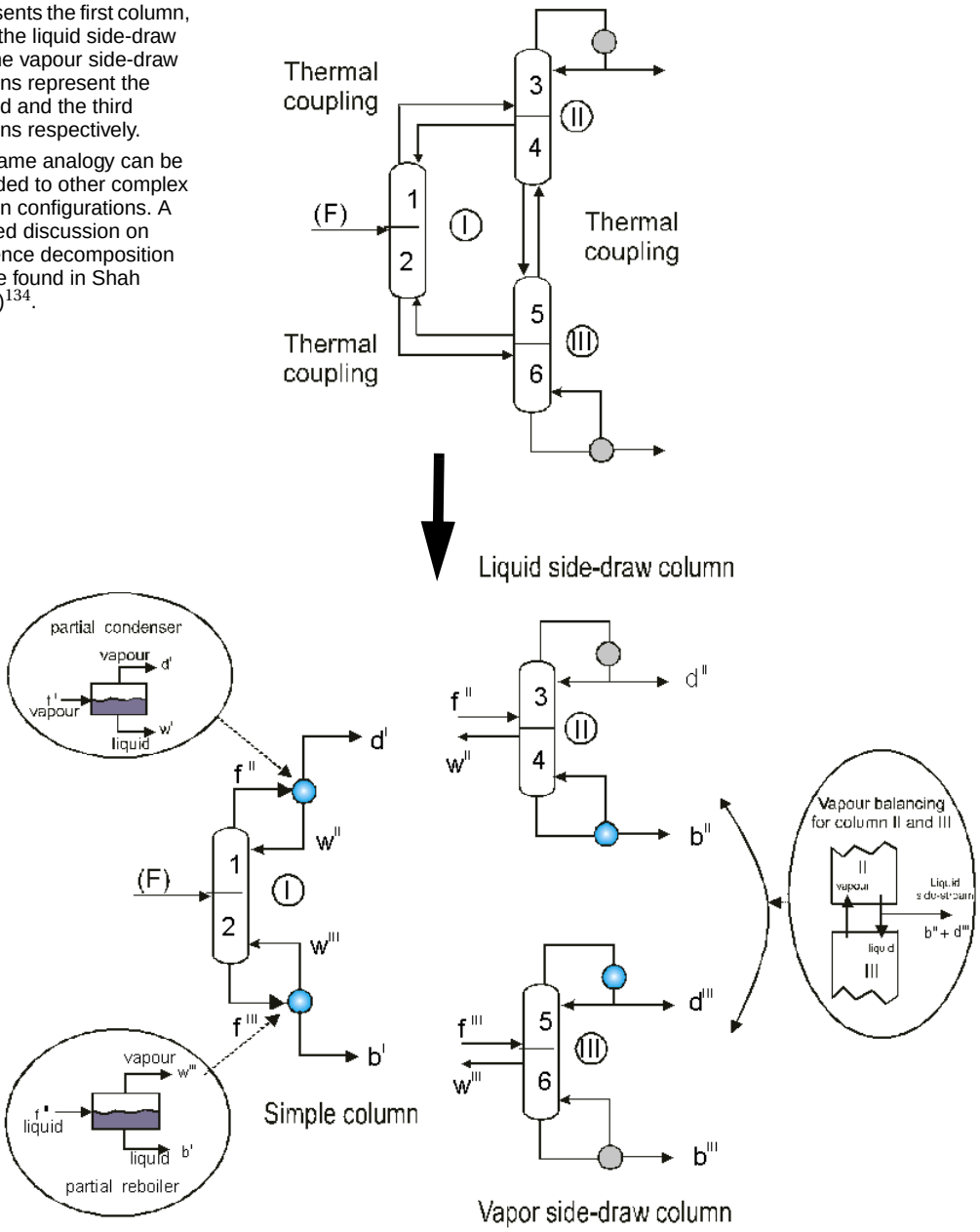
As discussed earlier, the fully thermally coupled distributed sequence results in the Petlyuk column (see **Figure 5.17**).

The sequence is further decomposed using the three types of simple columns as shown in **Figure 5.21**.

Figure 5.21

A simple column represents the first column, while the liquid side-draw and the vapour side-draw columns represent the second and the third columns respectively.

The same analogy can be extended to other complex column configurations. A detailed discussion on sequence decomposition can be found in Shah (1999)[134].



Different shortcut methods are employed on the basic simple columns to determine design parameters and the vapour-liquid traffic. The results of these calculations are reconciled and adjusted to represent the complex column configuration. In the next section, a brief summary of shortcut methods used to evaluate the distillation system is presented.

Shortcut Methods

The primary objective of the shortcut models here is to obtain the estimates for the vapour-liquid traffic (i.e., reflux and reboil ratios) and the number of trays in each section of the column.

- The minimum reflux ratio for the specified separation is calculated using Underwood method (Underwood, 1948[156]).
- The minimum number of theoretical stages are estimated using Winn's method (Kister, 1992[71]).
- The actual reflux and the number of stages are then determined by employing Molokanov's correlation (King, 1980[70]) for the specified R/R^{MIN} value.
- Triantafyllou and Smith (1992)[152] and Shah (1999)[134] discuss the extension of this method for the Liquid side-draw column and the Vapour side-draw column.

For more information regarding the methods used in the Shortcut model, refer to **Section 4.4.1 - Shortcut Method**.

All these methods make following two assumptions:

- Constant molar overflow (CMO).
- Constant relative volatility (CRV).

These assumptions restrict their applicability to the zeotropic systems. The geometric mean of relative volatilities from different sections is obtained to estimate a more realistic and representative set of volatility values that can be used in shortcut methods. However, it is recommended to carefully study the variation in relative volatilities values in different sections.

Reconciling Results

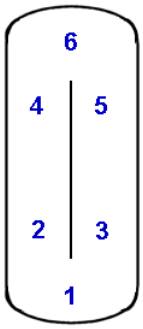
These design parameters are used with sizing and costing methods to obtain economic performance of the configuration. A detailed discussion of this can be found in Triantafyllou and Smith (1992)[152].

The design parameters obtained from the results of the basic simple columns are reconciled and adjusted to represent the actual complex column.

The vapour flow between the thermally coupled sections of the simple columns is balanced by removing condensers and/or reboilers from the

simple column sequence. Then the Molokanov equation is applied again to find the number of stages at the resulting value of the *RF* and the trays from different sections are added together to represent actual column shell. Finally, the temperatures and duties of all existing condensers and reboilers are estimated.

Operational Issues with Dividing Wall Column



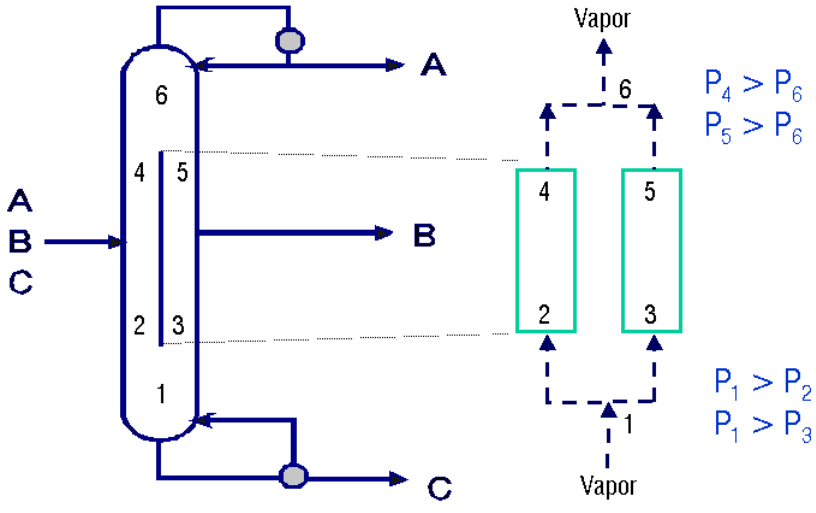
Sections of the Dividing Wall column.

The Dividing Wall column configuration consist of a single column with a wall that splits a section of the column into two. So the total number of sections in a Dividing Wall column is six.

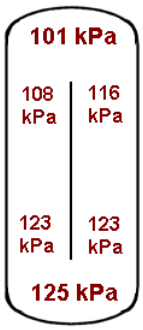
In order for the vapour to flow from the bottom of the column to the top of the column:

- The pressure in section 2 and 3 need to be less than the pressure in section 1.
- The pressure in section 4 needs to be less than the pressure in section 2.
- The pressure in section 5 needs to be less than the pressure in section 3.
- The pressure in section 6 needs to be less than the pressure in section 4 and 5.

Figure 5.22



For Dividing Wall column, the dividing wall may pose a problem. The wall in column creates two parallel paths for the vapour stream to flow in the column, thus allowing the potential for two different pressure differences in the paths.



Example

For example, a Dividing Wall column has a pressure of 125 kPa for section 1 and a pressure of 101 kPa for section 6. Section 2 and 3 has the same pressure of 123 kPa. The pressure in section 4 is 108 kPa and the pressure in section 5 is 116 kPa.

Both pressure values in section 4 and 5 are more than the pressure value in section 6. Unfortunately, the vapour split is harder to control and calculate, because section 2-4 has a pressure difference of 15 kPa and section 3-5 has a pressure difference of 8 kPa. The different value in pressure difference creates difficulties in the calculation/prediction the vapour flow rate.

To make calculation easier and faster, DISTIL always automatically change the pressure differences in the two section, so the pressure drop on both section 2-4 and section 3-5 are equal.

Adjusting Vapour Split Ratio

DISTIL allows you to equate the trays on two sides of the wall for both Dividing Wall and Petlyuk type columns. By equating the number of trays on both sides of the wall:

- You can adjust the vapour split ratio to 50:50. This may reduce the capital and operating cost of a condenser in the column design.

  For example, if the vapour split ratio of a column design is 15:85. One of the condenser is going to be very expensive and big to accommodate 85% of the vapour flow rate. While the other condenser is almost not be worth purchasing since it will handle only 15% of the vapour flow rate. By adjust the split ratio to 50:50, a reasonable value for both capital and operating costs are obtained.
- You can design a stable column structure. By creating equal number of trays on either side of the walls, the weight distribution in the column is equally spread out.

  For example, DISTIL may generate a the feasible column that produce the required product streams, but one side of the column has 10 trays, while the other side has 63 trays. So the number of

tray difference between the two sections/sides of the column is 53 trays. This large number differences will obviously cause problems when constructing the column and keeping the structure stable on the ground during a windy day.

For more information about the relationship between the reflux ratio and number of trays, refer to **Section 5.2.4 - Column Retrofit Options**.

To equate the number of trays on both side of the wall, DISTIL manipulates the reflux ratios of each section until the same number of trays is achieved.

For example, the vapour split ratio is 60:40 for a prefractionator with side draw. By decreasing the R/Rmin value on the prefrac side and/or increasing the R/Rmin value on the side-draw side, one can change vapour split ratio and manipulate the corresponding reboil ratios too. Reflux and reboil ratios are tied by mass balance and are directly proportional.

Lower R/Rmin value on the prefrac side will decrease the vapour flow on the prefrac side, while higher R/Rmin value on the side-draw side will increase the vapour flow on the side-draw side. This will result in bringing the vapour split ratio value closer to 50:50.

5.3.6 Sizing and Costing Methods

For more information about the sizing and costing methods, refer to **Chapter 9 - Size & Cost Assumptions**.

The shortcut model described in the previous section provides the necessary information from the column configuration to calculate the size and cost of the column design. DISTIL uses the temperatures from the condenser and reboiler to select the appropriate utility streams (based on the Pinch principles described by Linnhoff, 1993[97]) for the column design.

5.3.7 Modeling in Steady State Environment

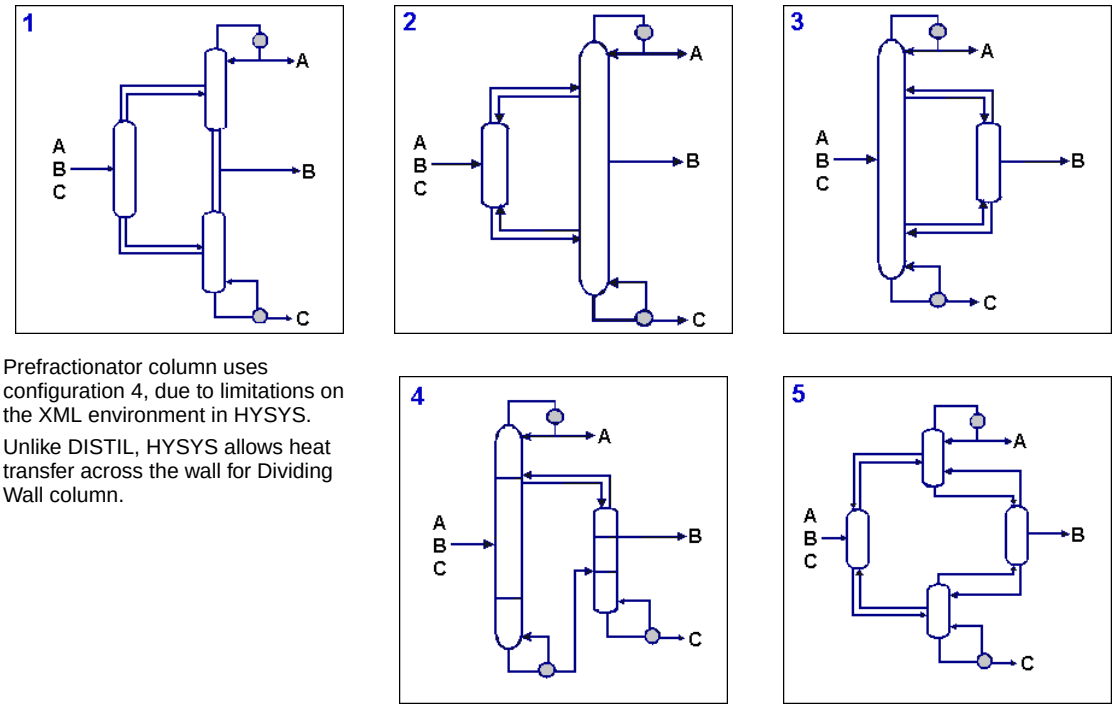
DISTIL allows you to export the complex column design into the HYSYS steady state environment.

To setup the column design in HYSYS, DISTIL:

- Populates a flowsheet in HYSYS with the column configuration
- Defines the connections between and/or within the columns
- Sets the columns at the optimum operating pressure
- Supplies the number of trays in different sections of the columns
- Supplies the estimates of temperatures, vapour-liquid traffic, reflux and reboil ratios, and compositions of the intermediate streams.

Depending on the type of column configuration you selected, HYSYS will use any one of the following five column configurations:

Figure 5.23



Prefractionator column uses configuration 4, due to limitations on the XML environment in HYSYS.

Unlike DISTIL, HYSYS allows heat transfer across the wall for Dividing Wall column.

5.3.8 Summary

Features

The summary of features available in the complex columns:

- Multi-component feed and products.
- On-line checks to detect azeotrope(s) in the system.
- Efficient and automatic product specifications using only light and heavy keys. It employs **Recovery Matrix** to describe multi-component products.
- Complete flexibility in selecting feasible key components through dynamic enumeration box.
- Computationally efficient approach to optimise recoveries of intermediate key components for different complex columns.
- Freedom to select the type of condenser(s) for the configuration.
- Complete flexibility in specifying operating condition. It can take pressure and/or temperature specifications in any section of the configuration and recalculate prevailing conditions in the remaining sections. It handles the pressure restrictions of different complex configurations.
- Accounts for the pressure drop with in-built logic to correct pressure drop that ensures the operability of the configuration.
- Improved logic to obtain the best set of relative volatility values.
- **Sensitivity Analysis** to study the variation in the performance parameter(s) of the configuration when operating pressure, R/Rmin, feed quality, and feed flowrate change in the specified range.
- Allows user to modify utility information, sizing data and capital costing coefficients (a default set of values is provided).
- Compare different complex configurations on Temperature-Enthalpy diagram.
- Seamless link between the Synthesis, Design and Analysis fronts.

Results & Output

The results and output values from the complex columns:

- Details of all products (flowrate, compositions, temperature, pressure, etc.).
- Optimum distribution of intermediate keys to minimize reflux ratio.
- Vapour-liquid traffic in each section of the configuration.
- Number of trays in each section of the configuration.
- Duties and temperatures of all condensers and reboilers of the configuration.
- Height and diameter of all column shells and Area of all heat exchangers.
- Capital, Operating and Total Annualized Cost of the each configuration.
- Comparison chart describing performance parameters for all complex configurations.

5.4 Column Sequencing

The following sections describe the background calculation/procedure performed by DISTIL to determine the optimum sequence of simple columns for separating multi-component feed stream into the desired products.

5.4.1 Separation Sequencing Problem

The multi-component feed stream is to be separated into a set of products (that can be multi-component in nature). In general, this can be done using number of feasible sequences of simple columns.

For example, one can separate the light product from the feed of each column (resulting in Direct Sequence) or successively separate heavy product (Indirect Sequence) or any other combinations of these two sequences.

The objective of this feature is to identify the most promising (based on the user-defined objective) sequences quickly with minimum process information from all feasible design options. This section first illustrates the importance of the sequencing problem and then defines the sequencing problem. A brief summary of supertask network and the optimization method (see Shah and Kokossis, 2002) is then provided.

5.4.2 Importance of Sequencing

As discussed before, a specified separation objective can be achieved by number of different sequences whose performance is substantially different. Look at the following cases to understand the importance of sequencing problem:

- Consider the feed stream containing light product that needs refrigeration for condensation. If that product is not separated in the beginning of the sequence then it will demand expensive refrigeration in more than one column and increase the operating cost.
- If the large fraction of the feed is comprised by a single product then delay in its separation adds the mass load on the downstream sequence increasing the separation cost and capital investment.
- Whenever a difficult separation (e.g., separation between isomers) is performed towards the beginning of the sequence the reflux (boil-up) load increases due to presence of all light (heavy) components resulting in fatter and more expensive columns.

From all these examples, it is clear that the decision about the sequence of splits has a big impact on the performance of the separation process. In most of the industrial processes, this decision is not obvious and needs careful screening and scoping. In the following sections, the details of the synthesis model and the optimization method is described.

5.4.3 Product Specifications

It is desired to separate a multi-component feed stream into n different products using distillation. The products can be pure components or multi-component mixtures. As the feed is separated into n products, user needs to specify n-1 splits.

All the components present in the feed stream are listed in order of decreasing volatility and are numbered from 1 to m. The products are arranged in order of increasing boiling points and are called products A to N. Each split is assumed to separate the feed stream into two products (viz. the top product and the bottom product) at the fixed pressure. The splits are arranged in the order of increasing top product temperature. (The split that separates the lightest product from the feed is called the first split.) One light and one heavy key characterize each

split.

The three-product system is defined by two splits called first and second split and requires the specification of two light keys (viz. *LK*1 and *LK*2) and two heavy keys (viz. *HK*1 and *HK*2).

The selection of key components obey the following equation to ensure the feasibility of the separation using distillation in the zeotropic systems where component order does not change with operating conditions.

$$1 \le LK_1 < HK_1 \le LK_2 < HK_2 \ldots \le \ldots LK_{n-1} < HK_{n-1} \le m \qquad (5.2)$$

where: 1, *m = the component indices of the first and the last components after arranging them in the order of decreasing volatility*

n = the number of different product streams in the separation system

The multi-component feed is separated into *n* different products using distillation. The products can be pure components or multi-component mixtures. Since the feed is separated into *n* products, the user needs to specify *n – 1* splits. The splits are defined using a light key and a heavy key. The information about the key components is used to fill the Recovery Matrix and define products completely. The details about the Recovery Matrix, key components and relevant assumptions can be found in **Section 5.3.3 - Specification of Three Product System**.

Unlike three products system, user needs to define the recoveries of all intermediate key components as well to define the products completely. It is important to note that one can not optimise the distribution of intermediate components in *n*-product system due to the technical limitations. The exact composition of products is then calculated from the recoveries. It is recommended to review the product composition before performing the sequence optimization. Any discrepancy in the product composition must be corrected either by modifying the key component or the component recoveries.

5.4.4 Representation

The definition of the feed and the products sets the stage for sequence optimization. This section describes the new synthesis and optimization framework employed here.

All the products of the separation system are arranged in the order of increasing boiling point and named A, B, C, etc. respectively with A as the lightest product. Each stream is represented by the products it carries while the distillation column is represented using a "/" between the products it separates from its feed stream.

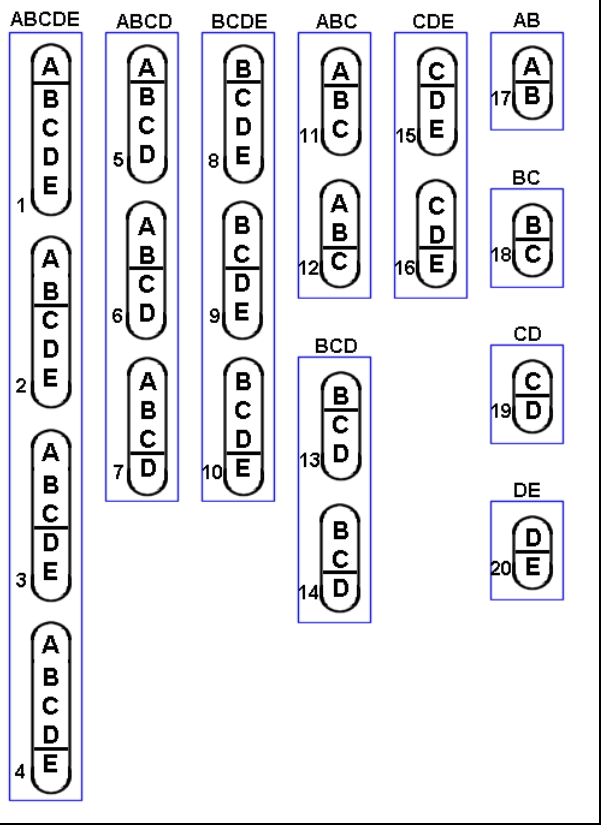
For example, in a five product system, A and E are the lightest and the heaviest products respectively and the feed stream is represented as "ABCDE". The column separating E from the main feed is represented by "ABCD/E" and the products of that column are "ABCD" and "E".

All possible column sequences are embedded in the synthesis superstructure using supertask representation (Shah & Kokossis, 2002[135]). The supertask representation assumes that the volatility order of the products do not change with the operating conditions. That is, the product A will be always lighter that product B and product B will be always lighter than C and so on. This means, at no point in the sequence the stream "BD" can exist you can have streams "BCD" or "BC" or "CD" but not "BD".

Based on the above assumption, it is possible to derive a set of all possible streams that can be potentially generated by all the columns of the separation sequence. These streams are then used to define the all potential splits using simple columns tasks in the synthesis representation.

The set of all streams and the tasks for a five-product system is shown in the figure below.

Figure 5.24



One can represent any sequence of splits by selecting a particular set of tasks from the supertask representation. For example, a direct sequence for the five-product system can be realized by selecting tasks 1, 8, 15 and 20 from the above figure.

The options related to operating conditions of the tasks are screened by introducing instances of the tasks. Instance of a task performs the same separation but operates at different pressure or with reflux flow. For example, the three instances of task “D/E” are shown in **Figure 5.24**. They all receive identical feed stream “DE” and they produce same products D and E but operate at different pressures. By introducing number of pressure levels, engineer can identify optimum pressure range for each column of the separation system.

The biggest advantage of this representation is that the number of tasks increase much slowly than the number of sequences especially when number of products or pressure levels increase (see the table below).

Number of Products	One Pressure Level		Two Pressure Level		Three Pressure Level	
	Tasks	Sequences	Tasks	Sequences	Tasks	Sequences
3	4	2	8	8	12	18
4	10	5	20	40	30	135
5	20	14	40	224	60	1134
6	35	42	70	1344	105	10206
7	56	132	112	8448	168	96228
8	84	429	168	54912	252	938223
9	120	1340	240	366080	360	9382230
10	165	4862	330	2489344	495	95698746

For example, in a eight-product system if we consider two-pressure levels then 54,912 distillation sequences are feasible, the supertask representation accommodates all these options using only 168 tasks and thus decreases the search efforts and improves computational performance.

The other advantage is that it defines feed and products of each task ahead of structural optimization and allows user to employ any performance model without introducing computational problems in optimization.

The supertask representation can be further extended to include options related to complex columns. User can refer to Shah & Kokossis, 2002[135] for further details.

5.4.5 Task Classification

The sequencing problem is very sensitive to the performance of the tasks included in the supertask representation. Hence it is important to assign promising values or more appropriate ranges of operating conditions to all tasks. To facilitate this process, DISTIL classify all tasks based on:

- **Instance number**: A set of all tasks that have identical instance number. That is the first instance of all tasks is grouped together in a set of first instances and so on. For example, if user defines two instances of all tasks then the set of second instances will include the second instance of all the tasks.
- **Splits**: A set of all tasks that perform an identical split. For example, in a five-product system, tasks AB/CDE, AB/CD, B/CDE, AB/C, B/CD and B/C perform a same split although they receive different feeds and/or produce different products. They will be grouped under split –B/C--.
- **Feed stream**: A set of all tasks that receive an identical feed stream. For example, in a five-product system, tasks A/BCDE, AB/CDE, ABC/DE and ABCD/E receive the same type of feed stream although they perform different splits and produce different products. They will be grouped under feed stream type ABCDE.
- **Top product stream**: A set of all tasks that produce an identical top product stream. For example, in a five-product system, tasks B/CDE, B/CD, and B/C produce the same type of top product stream although receive different feed streams. They will be grouped under top-product stream type B.
- **Bottom product stream**: A set of all tasks that produce an identical bottom product stream. For example, in a five-product system, tasks AB/C and B/C produce the same type of bottom product stream although receive different feed streams. They will be grouped under bottom-product stream type C.

user can use only one classification at a time. It is not possible to mix and match due to overlapping sets.

Using this classification user can assign appropriate conditions to address correct tradeoffs. Following example illustrates this idea more clearly.

1. In the sub-ambient separations (low temperature), the column operating pressure is decided from the available refrigeration levels (or in other words, condenser temperature) then its useful to classify tasks using top products. This ensures that all the tasks producing identical top-products will operate at same pressure and allow DISTIL to make structural decisions about the sequence more accurately.
2. When the site has limited levels of hot utilities, it is necessary to adjust pressure levels using reboiler temperatures then the tasks are classified using bottom-products of the tasks.

3. When the splits need to be performed at particular pressures (irrespective of condenser or reboiler temperatures) as in case of isomer separations then its desired to classify tasks using splits.

Consider a five-product system where operating condition is bracketed using 3 instances to understand the classification criteria. Task classification and all the sets for this example are listed below.

- **Instance number**: It will have three instances of all tasks.

Number	Instance	Tasks
1	1	All the tasks
2	2	All the tasks
3	3	All the tasks

- **Splits**: Four splits are necessary for produce five products. The tasks involved in each split are listed below.

Number	Split	Tasks
1	A/B--	A/BCDE, A/BCD, A/BC, A/B
2	--B/C--	AB/CDE, AB/CD, AB/C, B/CDE, B/CD, B/C
3	--C/D--	ABC/DE, ABC/D, BC/DE, BC/D, C/DE, C/D
4	--D/E	ABCD/E, BCD/E, CD/E, D/E

- **Feed stream**: The set all the feed streams for this example and the associated task is listed below.

Number	Feed Stream	Tasks
1	ABCDE	A/BCDE, AB/CDE, ABC/DE, ABCD/E
2	ABCD	A/BCD, AB/CD, ABC/D
3	BCDE	B/CDE, BC/DE, BCD/E
4	ABC	A/BC, AB/C
5	BCD	B/CD, BC/D
6	CDE	C/DE, CD/E
7	AB	A/B
8	BC	B/C
9	CD	C/D
10	DE	D/E

- **Top product stream**: The set all top product streams for this example and the associated task is listed below.

Number	Top-Product Stream	Tasks
1	ABCD	ABCD/E
2	ABC	ABC/DE, ABC/D
3	BCD	BCD/E
4	AB	AB/CDE, AB/CD, AB/C
5	BC	BC/DE, BC/D
6	CD	CD/E
7	A	A/BCDE, A/BCD, A/BC, A/B
8	B	B/CDE, B/CD, B/C
9	C	C/DE, C/D
10	D	D/E

- **Bottom product stream**: The set all bottom product streams for this example and the associated task is listed below.

Number	Bottom-Product Stream	Tasks
1	BCDE	A/BCDE
2	BCD	A/BCD
3	CDE	AB/CDE, B/CDE
4	BC	A/BC
5	CD	AB/CD, B/CD
6	DE	ABC/DE, BC/DE, C/DE
7	B	A/B
8	C	AB/C, B/C
9	D	ABC/D, BC/D, C/D
10	E	ABCD/E, BCD/E, CD/E, D/E

5.4.6 Modeling of Task

All the tasks are modeled as the simple columns that receive one feed and produce two products. The details of the performance models of the simple tasks can found in **Section 5.2.1 - Performance Models**. The user-specified objective for each task is then generated and used in the structural optimization. The complete MILP model is described in the next section.

5.4.7 MILP Formulation

The synthesis problem is formulated into an optimization problem with the use of the following sets, parameters and variables:

- Sets

  $T = \{t \mid t \in T \text{ is a simple task}\}$

  $M = \{m \mid m \in M \text{ is a stream type}\}$

  $T^{fr} = \{t \mid t \in T \text{ receives fresh feed}\}$

  $T^{int} = \{t \mid t \in T \text{ receives intermediate feed}\}$

  $T_m^{inp} = \{t \mid t \in T^{int} \text{ receives stream } m \in M\}$

  $T_m^{out} = \{t \mid t \in T^{int} \text{ produces stream } m \in M\}$

- Parameters

  $\zeta_{m,t}$ = feed fraction yielding stream $m \in M$ in $t \in T$

  F_t = nominal feed flowrate of $t \in T$

  F^{tot} = total feed flowrate

  Obj_t^{Nom} = objective value of the task at the nominal flow value $t \in T$

- Variables
  The variables include discrete and continuous variables defined by

  Y_t = binary variables for the existence of $t \in T$

  f_t = feed flowrate of $t \in T$

  Obj_t = objective value of the task $t \in T$

Constraints of the Synthesis Problem

These include simple material balances and the expressions related to the objective value. The logical constraints associate continuous and integer variables.

They are mass balances for the tasks,

$$F^{tot} - \sum_{k \in T^{fr}} f_k = 0 \tag{5.3}$$

$$\sum_{t \in T} (\zeta_{m,t} \times f_t) - \sum_{k \in T_m^{inp}} f_k = 0 \qquad \forall m \in M \tag{5.4}$$

expression for the objective,

$$Obj_t = Obj_t^{Nom} \times \frac{f_t}{F_t} \qquad \forall t \in T \tag{5.5}$$

and logical constraints.

$$f_t - F_t \times Y_t \leq 0 \qquad \forall t \in T \tag{5.6}$$

A set of contingency constraints improves the branching in the optimization.

$$Y_t - \sum_{k \in T_m^{out}} Y_k \leq 0 \qquad \forall t \in T_m^{inp}, m \in M \tag{5.7}$$

The proposed cost model predicts the cost of each task for its nominal flowrate (F) hence it is scaled linearly using a feed fraction (f/F) to predict the cost of the task at the prevailing flowrate f.

Synthesis Objective

The objective function can be stated so that the optimise is either:

- Economic objectives (i.e., minimize overall separation cost, maximise profit)
- Efficiency based objectives (i.e., maximize the thermodynamic or the separation efficiency).

The typical objective function for the case (where economic is the objective) takes the form:

$$\text{Synthesis Objective} = \sum_{t \in T} Obj_t \tag{5.8}$$

Solution

In all cases, the formulation involves only linear expressions of continuous (i.e., flowrates) and binary variables (i.e., existence of task) that give rise to an MILP problem. It is solved using XPRESS or LPSOLVE.

5.4.8 Retrofit Options

Pressure Optimization

The MILP performs the structural optimization and identifies the optimum range of column pressure during the sequencing stage. The further fine-tuning of the operating pressure is performed here by identifying the utility change points in the bracketed range for each column of the sequence. The further details of the pressure optimization of a column can be found in **Section 5.2.3 - Optimising Column Pressure**.

Asset Utilization

The objective of this feature is to evaluate promising sequences that use available assets. It allows user to specify available column shells in the form of number of trays and then performs structural optimization to identify the best sequence that can employ all or most of the column shells with minimum operating cost.

In this scenario, tasks are classified using splits and then user provides a column shell for each split. This allocates the column shell to each split and hence each task but the sequence of split is not yet identified. At this point, the number of trays available for each task is known. As long as these trays are greater than its minimum stages, reflux ratio of the task is modified to perform the separation in available number of stages (refer to **Section 5.2.4 - Column Retrofit Options** for more information). In this manner, each task adjusts its operating reflux to utilize allocated column shell. The structural optimization of reflux-adjusted tasks is then performed to minimize the operating cost.

This feature is extremely useful in debottle-necking of separation sequences. Also when the column internals are changed or modified one can re-evaluate the promising sequence to save energy cost.

6 Heat Integration - Pinch Analysis

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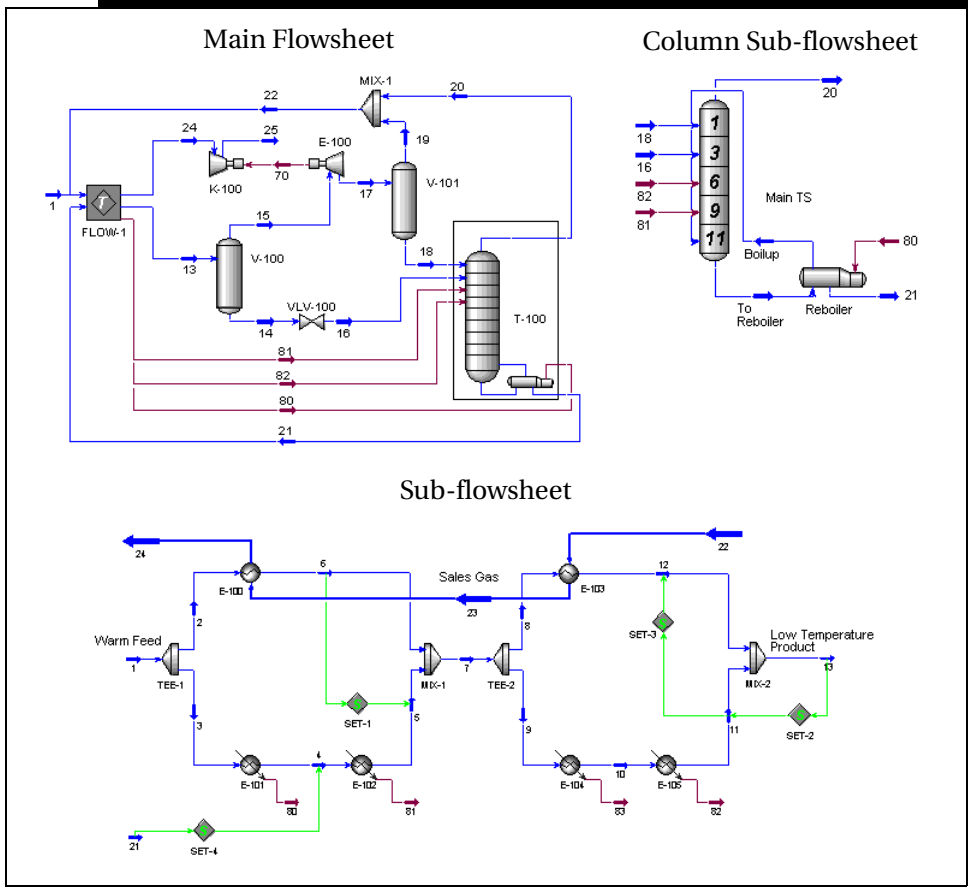
6.1 Introduction

Heat integration in HX-Net is designed for analysing and improving the performance of heat exchanger networks (HEN). HX-Net focus on analysing the networks from operations' as well as design's point of view.

For example, consider the PFD of a process in the figure below.

Figure 6.1



In the above process, heat is exchanged in five process-process exchangers (i.e., *Ex-100*, *Ex-101*, *Ex-103*, *Ex-104*, and *Ex-105*) and there is one cooler (*Ex-102*). The cooler uses 0.9 MW of refrigerant energy to perform the cooling.

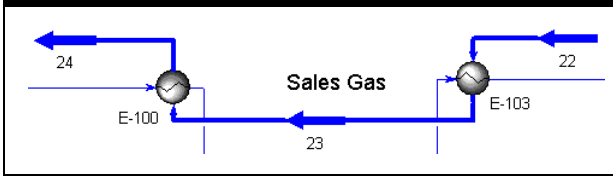
A few questions that one could ask when analysing a process are:

- Does the process really need the five heat exchangers or could the process do with less?
- Does the process really need 0.9 MW of refrigerant or could the process do with less?
- What is the minimum amount of heat transfer area that the process requires?

These and similar questions would be asked by an engineer critically analysing the HEN design. This chapter will introduce you to the tools that HX-Net provides to help one answer such questions.

If the PFD in **Figure 6.1** is examined closely, you will notice that the Sales Gas stream is being heated from $-92.49°C$ to $-8.002°C$ in exchanger E-103. The Sales Gas stream is further heated to $24.86°C$ in exchanger E-100.

Figure 6.2



Thus there is a requirement of heating 4375 kg/hr of Sales Gas from $-92.49°C$ to $24.86°C$. This is equivalent to a heating requirement of 5.6 MW. This can be represented as:

Figure 6.3

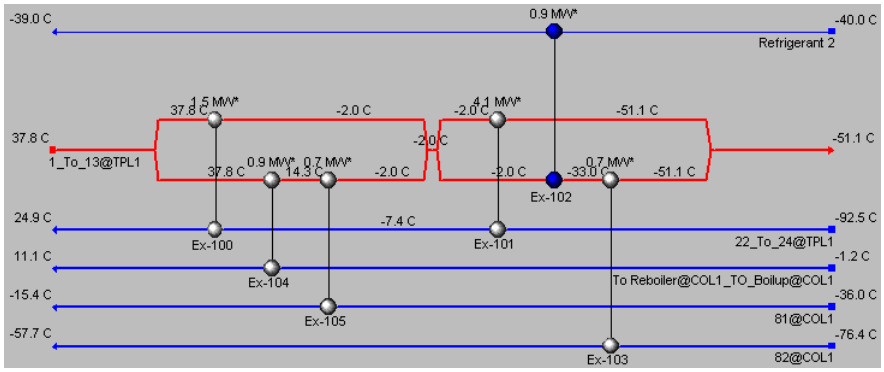
Similarly, the cooling requirements for the Warm Feed stream from $37.76°C$ to $-51.11°C$ can be represented as:

Figure 6.4

If all the heating and cooling requirements of the process were bundled together, the result is the Grid Diagram. Simplistically, the Grid Diagram is an overview of all the heating/cooling requirements of the process. A detailed description of the Grid Diagram will be made later in Section 6.2.7 - Grid Diagram.

For the PFD in consideration, Figure 6.1, the following heat exchanger network (HEN) design is formed.

Figure 6.5



The following table display the list of process streams in the Grid Diagram and the material streams from the PFD that make up the process streams.

Process Stream in HEN	Material streams from PFD
1_to_13@TPL1	Material streams 1, 2, 3, ... 12, 13 in the Sub-flowsheet. The inlet temperature is from material stream 1, and the outlet temperature is from material stream 13.
22_to_24@TPL1	Material streams 22, 23, and 24 in the Sub-flowsheet. The inlet temperature is from material stream 22, and the outlet temperature is from material stream 24.
ToReboiler@COL1_to_ Boilerup@COL1	Material streams To Reboiler and Boilup in the Column sub-flowsheet. The inlet temperature is from material stream To Reboiler, and the outlet temperature is from material stream Boilup.
81@COL1	Side condenser on tray 5 in the Column sub-flowsheet. The inlet temperature is from stream in tray 5, and the outlet temperature is from stream in tray 6.
82@COL1	Side condenser on tray 8 in the Column sub-flowsheet. The inlet temperature is from stream in tray 8, and the outlet temperature is from stream in tray 9.

In the Column Sub-flowsheet of Figure 6.1, there are two energy streams (81 and 82) entering tray 6 and 9.

These energy streams represent heat being transferred into the streams in the trays, thus indicating there are heat exchangers attached to tray 6 and 9.

The following section discuss the basic terminology that is necessary to understand in order to make use of the pinch analysis tools.

6.2 Basic Terminology

In order to build a heat exchanger network (HEN), a number of variables must be known. The variables are information about all streams containing energy, such as process and utility streams, and the economic parameter that will govern the cost calculations.

The following sections will describe in detail the basic terminology of the required variables used to make up a HEN.

6.2.1 Process Streams

Process streams are streams containing the fluid you want to heat or cool. As a minimum, HX-Net requires you to specify the name of the process stream, inlet temperature, outlet temperature, and MCp or Enthalpy.

Refer to **Section 6.1 - Introduction** for more information on what is considered a process stream in a plant flowsheet.

An example of a process stream is the Sales Gas stream (material streams 22, 23, and 24) from the PFD in **Figure 6.1**. This process stream is heated from -92.49°C to 24.86°C, and has an enthalpy change of 5.6 MW associated with it.

MCp Parameter

MCp is the product of the specific heat capacity of the process stream (Cp) and the mass flow rate of the process stream. The following equation is used to calculate MCp:

$$MCp = \frac{dH}{dT} \tag{6.1}$$

where: dH = the incremental change in enthalpy of the process stream

dT = the incremental change in temperature of the process stream

For more information, refer to **Section 6.2.4 - Segmenting Streams**.

The MCp of a stream seldom varies when the temperature difference is not great. However, for larger temperature difference you should segment the stream at different range of temperature to accurately portray the MCp value of the stream as it is heated or cooled.

Enthalpy Parameter

As the process stream enters and exits the heat exchanger network, the stream enthalpy changes:

- For process streams being heated, the enthalpy change is the total duty required to heat the stream from its supply temperature to the target temperature.
- For process streams being cooled, the enthalpy change is the total duty required to cool the stream from its supply temperature to the target temperature.

Other Parameters

The following table lists and describes other parameters used to modify the stream so that it closely match the process stream in an actual plant:

Parameter	Description
HTC	The local heat transfer coefficient associated with the individual stream. The default heat transfer coefficient is 720 kJ/hm^{2}C (35.22 Btu/hft^{2}F).
Flowrate	The mass flow rate of the process stream.
Effective Cp	The specific heat capacity of the stream. HX-Net calculates this value once the above mentioned minimum variables and a flow rate has been specified.
DT Cont.	This is the minimal approach temperature associated with the stream. HX-Net assumes a default value of 10^{o}C.

Hot and Cold Process Streams

The process streams in a heat exchanger network can be categorize into two types:

Cold Stream icon

Hot Stream icon

- **COLD.** A cold process stream is heated up in the heat exchange network. The inlet temperature of a cold process stream is lower than the outlet temperature.
- **HOT.** A hot process stream is cooled down in the heat exchange network. The inlet temperature of a hot process stream is higher than the outlet temperature.

HX-Net determines the type of stream based on the inlet and outlet temperature of the process stream.

6.2.2 Utility Streams

Utility streams are streams containing the heating or cooling fluid generated by utilities.

Utility streams are used to satisfy unsatisfied heating and/or cooling requirements of the process streams.

Most simulation programs, like HYSYS, do not have a concept of utilities. They simply use heaters/coolers to satisfy some heating/cooling demand.

As a minimum, it is necessary to specify the utility stream's name, inlet temperature, and outlet temperature. In addition, you must enter the cost per energy of the utility if you want to calculate the operating cost of the heat exchanger network. The above information requirements are only necessary if you want to enter your own utility stream.

Refer to **Section 10.2 - Utility Database View** from the **User Guide** for more information.

HX-Net supplies a list of default utilities you can select from which has all the information you need. One can configure their own set of default utilities if required.

Creating a Utilities Database

To create a utility database for future use:

The *Utility Database* button is usually located in the *Options* tab/page of the property view.

1. Access the Utility Database view by clicking the **Utility Database** button.
2. Modify the utility information to suit your simulation case.

Save Default Utilities to File icon

3. Click the **Save Default Utilities to File** icon to access the Save Heat Integration Defaults view.
4. Enter a name for the new utilities database file and select a location to store the file.
5. Click the **Save** button to save the utility database as a *.hud file. Refer to **Section 10.2 - Utility Database View** from the User Guide for more information.

Other Parameters

The following table lists and describes other parameters used to modify the utility stream so that it closely match the utility in an actual plant:

Matrix Column	Description
HTC	The local heat transfer coefficient associated with the individual stream. HX-Net supplies a default heat transfer coefficient value of 720 kJ/hm^{2}C (35.22 Btu/hft^{2}F).
Target Load	HX-Net calculates the Target Load of the utility stream that satisfies the process stream temperature requirements in the heat exchanger network. The Target Load is the total enthalpy change of the utility stream. A cold utility stream is heated in the heat exchanger network. A hot utility stream is cooled in the heat exchanger network.
Effective Cp	The specific heat capacity of the stream. HX-Net calculates this value once the above mentioned minimum variables and a flow rate has been specified.
Target Flowrate	The required flow rate for the utility stream based on the calculated Target values.
DT Cont.	This is the minimal approach temperature associated with the stream. HX-Net assumes a default value of 10^{o}C.

Refer to **Section 6.3 - Targets** for more information regarding the Target values.

Hot and Cold Utility Streams

The utility streams in a heat exchanger network can be categorize into two types:

Cold Stream icon

Hot Stream icon

- **COLD.** A cold utility stream is heated up in the heat exchange network. The inlet temperature of a cold process stream is lower than the outlet temperature.
- **HOT**. A hot utility stream is cooled down in the heat exchange network. The inlet temperature of a hot process stream is higher than the outlet temperature.

6.2.3 Hot and Cold Status Bars

HX-Net uses status bars at the bottom of the operation's view to indicate whether there is sufficient cold /hot utilities in the HEN design for the process streams being cooled/heated to achieve the specified outlet temperature.

There are three possible status:

- **Sufficient**. The temperatures of the utility streams are cool enough or hot enough to satisfy the cooling and heating demands of the system respectively. The colour of the status bar is green.
- **Insufficient**. The temperatures of the utility streams are not cool enough or hot enough to satisfy the cooling and heating demands of the system, respectively. The colour of the status bar is red.
- **Cross Pinch**. The outlet temperature of any cold utility stream(s) is higher than the cold pinch temperature, or the outlet temperature of any hot utility stream(s) is lower than the hot pinch temperature. The colour of the status bar is yellow. The utility can or cannot be sufficient.

6.2.4 Segmenting Streams

While performing a pinch analysis, it is necessary to linearize the enthalpy changes in the streams.

This is due to the fact that some of the computations are quite intensive. Obtaining reliable results in a reasonable time frame forces HX-Net to make some simplifying assumptions like this one.

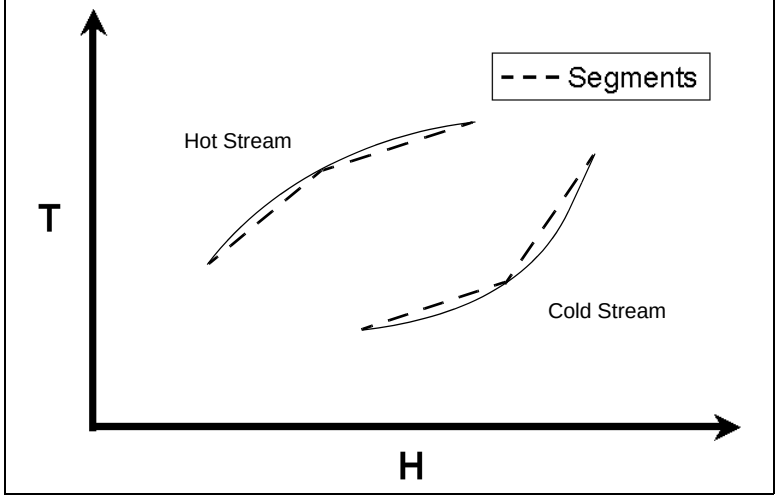
A constant specific heat capacity can be a good approximation for the behavior of a stream if the change in heat capacity, MCp, is small.

Segmenting a stream becomes necessary when the heat capacity of a stream is not constant over its temperature range across the heat exchanger network (HEN). Large variations in heat capacity can result from a phase change in the stream.

Segmenting Process Streams

As shown by the figure below, the type of process stream determines how it is segmented.

Figure 6.6



To preserve a conservative approach, hot process stream segments must always predict a lower temperature than the actual temperature. Likewise, cold process stream segments must always predict a temperature higher than the actual temperature.

You can segment a process stream by defining different heat capacities and local heat transfer coefficients for different temperature ranges of the temperature-enthalpy plot.

Segmenting Utility Streams

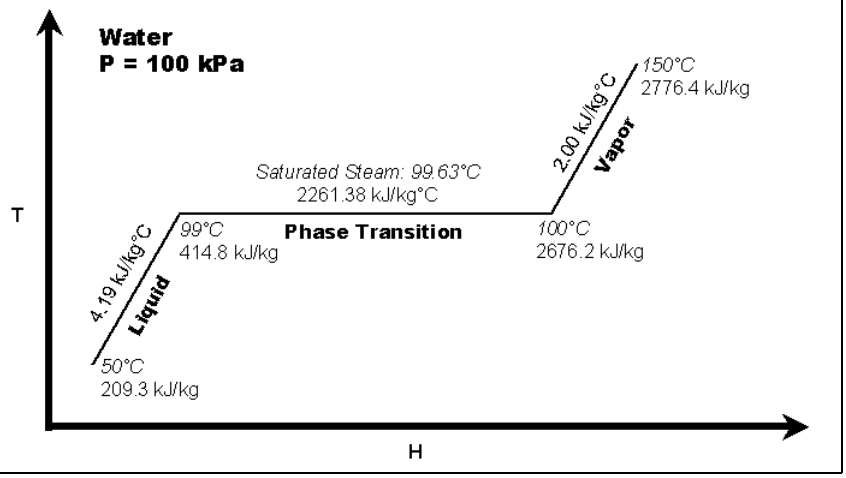
A constant specific heat capacity can be a good approximation for the behaviour of a utility stream if the change in Cp is small. However, it can be necessary to segment a utility stream if its heat capacity changes significantly over its temperature range.

For instance, if superheated steam is used as a hot utility stream, it can condense in the heat exchanger network. You can model this phase change by dividing the utility stream into three segments: the cooling of the superheated steam, the condensing of the steam, and the cooling of the condensate. Each segment has a different Cp associated with it. The phase change can be modelled using a very large Cp.

You can segment a utility stream by defining different specific heat capacities and local heat transfer coefficients for different temperature ranges of the temperature-enthalpy plot.

The figure below, displays a utility stream going from 50°C to 150°C at 100 kPa. The utility stream is modelled having three segments with a phase transition at 100 kPa.

Figure 6.7



The first one models liquid water enthalpy behaviour from 50°C to 99°C with an average Cp of 4.19 kJ/kg°C. The second one models the phase change of water in terms of specific heat. The assumption is that the

water phase transition takes place between 99°C and 100°C. This assumption is considered quite good considering that saturated vaporized water temperature at 100 kPa is 99.63°C. The average Cp for that segment is 2261.38 kJ/kg°C. The third segment models vapor water enthalpy behaviour from 100°C to 150°C with an average Cp of 2.00 kJ/kg°C.

6.2.5 Heat Transfer Coefficient

There are three ways to specify the heat transfer coefficient (HTC) of a process or utility stream in the heat exchanger network.

Manual Input

You can specify the HTC value for a process or utility stream:

1. Do one of the following:
   - Access the **Process/Utility Streams** tab in the HIC view.
   - Access the **Process/Utility Streams** page in the HIP view.
2. Select the cell in the **HTC** column associated to the stream you want to manipulate.
3. Enter the new HTC value in the selected cell.

Based on Physical Properties

You can provide physical property values and have HX-Net calculate the HTC value based on the specified property values:

1. Do one of the following:
   - Access the **Process/Utility Streams** tab in the HIC view.
   - Access the **Process/Utility Streams** page in the HIP view.
2. Open the Stream view of the stream you want to modify, by double-clicking in any of the cells (except HTC cell) in the row associated to the stream.
3. On the Stream view, go to the **Physical Properties** tab.

Refer to **Chapter 6 - Stream View** from the **Heat Integration** manual for more information about the Stream view.

4. Enter the values for the following physical properties: viscosity, conductivity, density, and specific heat capacity.

HX-Net requires a value for all the above mentioned physical properties in order to calculate the HTC value.

This is a representative value for the entire stream.

Notice the stream could flow through several exchangers and the individual velocity through each exchanger could be different.

5. Enter the value of a representative tube and shell side velocity and flow area diameter.
6. With the previous mentioned information, HX-Net calculates a value for HTC.
   This value is a good representative value that could be used to perform further calculations.

The goal at this point of the procedure is to obtain a top-level view of the heating-cooling requirements. The accuracy that the above mentioned values provide is good enough for this purpose.

The following are the equations used to calculate the HTC value based on the specified variable values.

For shell side (hot stream):

For shell side (hot stream):

$$\frac{h \times D}{k} = 0.36 Re^{0.55} \times Pr^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{6.2}$$

For tube side (cold stream)

$$\frac{h \times D}{k} = 0.023 Re^{0.80} \times Pr^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{6.3}$$

Reynolds Number:

$$Re = \frac{D \times \rho \times \nu}{\mu} \tag{6.4}$$

Prandtl Number:

$$Pr = \frac{Cp \times \mu}{k} \tag{6.5}$$

Assume:

$$\left(\frac{\mu}{\mu_w}\right)^{0.14} = 1 \tag{6.6}$$

where: h = *the heat transfer coefficient*

D = *the flow area diameter*

k = *the thermal conductivity*

ρ = *the stream density*

ν = *the stream velocity*

μ = *the stream viscosity*

Cp = *the effective specific heat*

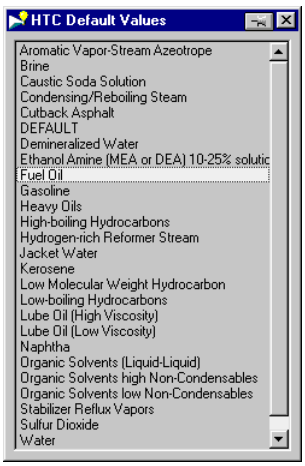
The calculated value of the HTC is representative for the entire stream that could flow through several heat exchangers.

HTC Database

You can select the HTC value from the HTC database:

1. Do one of the following:
   - Access the **Process/Utility Streams** tab in the HIC view.
   - Access the **Process/Utility Streams** page in the HIP view.
2. Double-click on the cell in the **HTC** column associated to the stream you want to manipulate. The HTC Default Values view appears.

Figure 6.8



3. Select the HTC value you want and click the **Close** icon to close the HTC Default Values view.

The list of default HTC values can be modified in the HTC Database view, refer to **Section 1.3 - HTC Database** from the **Heat Integration** manual for more information.

6.2.6 Economic Parameters

The economic parameters are required to calculate the capital cost and the annualization factor of the heat exchangers in the heat exchanger network (HEN). The economic parameters varies depending on the type of heat exchanger is used in the HEN.

Types of Heat Exchanger

There are two types of heat exchangers in this program. Each type has its own equation/formula for calculating the capital cost.

- Heat Exchanger. This option considers the Shell and Tube type exchangers, which uses convection to transfer energy. The capital cost is based on the heat transfer area.
- Fired Heater. This option considers the fired heater type exchangers, which uses radiation to transfer energy. The capital cost is based on the duty/amount of energy that needs to be transferred.

Material of Construction

A typical HEN will have multiple heat exchangers, and there may be different material used to construct the heat exchangers.

Refer to the following **Basic Economic Parameters** section for more information about capital cost.

You can indicate that a heat exchanger construction material is different by selecting a different set of economic parameter values (used to calculate the capital cost of the exchanger) to be associated to the heat exchanger.

HX-Net allows you to have multiple sets of economic parameter values, and allows you to select/assign the different cost set to certain heat exchangers in the HEN.

To create a cost set:

1. Do one of the following:
   - Access the **Economics** tab in the HIC view.
     Refer to **Section 2.2.3 - Economics Tab** from the **Heat integration** manual.
   - Access the **Economics** page in the HIP view.
     Refer to **Section 4.4.1 - Data Tab** from the **Heat Integration** manual.
2. Enter the following information for the cost set:
   - Name of the cost set, like **CS - Material** or **SS - Material**.
   - Installation and purchase cost of the heat exchanger.
   - Duty-related or area-related cost law coefficients of the heat exchange unit.
3. Select the heat exchanger type. HX-Net contains two types: shell & tube and fired heater.

HX-Net provides a default cost set based on a shell & tube type exchanger with carbon steel as the construction material.

To assign a different cost set to a hot-cold stream pair, refer to **Section 1.4 - Matchwise Economic View** from the **Heat Integration** manual.

Basic Economic Parameters

The basic economic parameters used to calculate the cost of the heat exchanger network are grouped into three cost sets: capital cost, operating cost, and total annualized cost (TAC).

Capital Cost

The capital cost is the fixed cost for purchasing and installing the heat exchanger(s). As mentioned before, HX-Net provides two types of heat exchangers: shell & tube and fired heater. Each type of heat exchange equipment has their own equation for calculating the capital cost:

Shell & Tube:

$$CC = a + b\left(\frac{Area}{N_{shell}}\right)^{c} \times N_{shell} \tag{6.7}$$

Fired Heater:

$$CC = a + b(Duty)^{c} \tag{6.8}$$

where: CC = the installed capital cost of a heat exchanger ($)

a = the installation cost of the heat exchanger ($)

b,c = the duty/area-related cost set coefficients of the heat exchanger

Area = the heat transfer area of the heat exchanger

N_{shell} *= the number of heat exchanger shells in the heat exchanger*

Duty = the amount of energy being transferred in the heat exchanger

If the unit set (variable units) have been changed and a script using a different unit set is played, there will be a problem with parameter *b*.

The reason for the problem is that *b* is not completely unitless. HX-Net does not handle (make changes to) the specified value, when the units change.

Operating Cost

The operating cost is a time dependent cost that represents the energy cost to run the equipment. For HX-Net, the operating cost is dependent on the calculated energy targets in the HEN. :

$$OC = \sum(C_{hu} \times Q_{hu,min}) + \sum(C_{cu} \times Q_{cu,min}) \quad (6.9)$$

where: OC = the operating cost ($/yr)

C_{hu} *= the utility cost for hot utility ($/ kW yr)*

$Q_{hu,min}$ *= the energy target of hot utility (kW)*

UC_{cu} *= the utility cost for cold utility ($/ kW yr)*

$Q_{cu,min}$ *= the energy target of cold utility (kW)*

Total Annualized Cost

The TAC accounts for both the capital cost and operating cost associated with the heat exchangers in the HEN. The equation below is used to calculate the TAC:

$$TAC = \Lambda \times \sum CC + OC \quad (6.10)$$

where: CC = the installed capital cost of a heat exchanger ($)

OC = the operating cost ($/yr)

Λ = the annualization factor (1/yr)

The annualization factor accounts for the depreciation of capital cost in the plant. It must be considered since the capital cost and operating cost of a heat exchanger network do not have the same units.

The equation below is used to calculate the annualization factor:

$$\Lambda = \frac{\left(1 + \frac{ROR}{100}\right)^{PL}}{PL} \qquad (6.11)$$

where: ROR = the rate of return (percent of capital)

PL = the plant life (yr)

For more information about total cost minimization, refer to **Section 6.3.6 - Range Targeting**.

It is usually the goal of the design engineer to minimize the total annualized cost of the plant.

Creating an Economic Database

HX-Net has a default economic database file called *ecodatabase.hcc*.

HX-Net recommends you do not save over the default database file.

If you created multiple economic sets for calculating the capital cost of the heat exchangers, HX-Net allows you to save the sets in an economic database.

To save an economic database file:

1. Do one of the following:
   - Access the **Economics** tab in the HIC view.
     Refer to **Section 2.2.3 - Economics Tab** from the **Heat integration** manual.
   - Access the **Economics** page in the HIP view.
     Refer to **Section 4.4.1 - Data Tab** from the **Heat Integration** manual.
2. Click the **Save Heat Exchanger Capital Cost Parameters to file** icon. The Save Heat Integration Defaults view appears.
3. Select a location to save the economic database using the **Save in** drop-down list.
4. Enter a name for the economic database in the **File name** field.

Save Heat Exchanger Capital Cost Parameters to file icon

5. Click the **Save** button.
   The economic database file extension is ***.hcc**.

To access an economic database file:

1. Do one of the following:
   - Access the **Economics** tab in the HIC view.
     Refer to **Section 2.2.3 - Economics Tab** from the **Heat integration** manual.
   - Access the **Economics** page in the HIP view.
     Refer to **Section 4.4.1 - Data Tab** from the **Heat Integration** manual.
2. Click the **Open Saved Heat Exchanger Capital Cost Parameters** icon. The Open Heat Integration Defaults view appears.

Open Saved Heat Exchanger Capital Cost Parameters icon

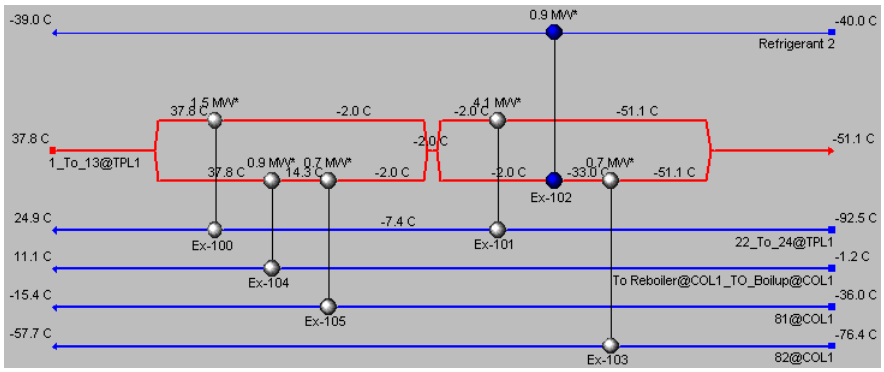
3. Locate and select the economic database file you want using the **Look in** drop-down list.
4. Click the **Open** button.

6.2.7 Grid Diagram

Refer to **Section 6.1 - Introduction** for information on how the streams in a PFD associate with process streams in a Grid Diagram.

The Grid Diagram is an image that displays how individual process and utility streams are matched with one another using heat exchangers. This image helps portray the heat exchanger network (HEN) design in a format that is easier to manipulate and see the results.

Figure 6.9



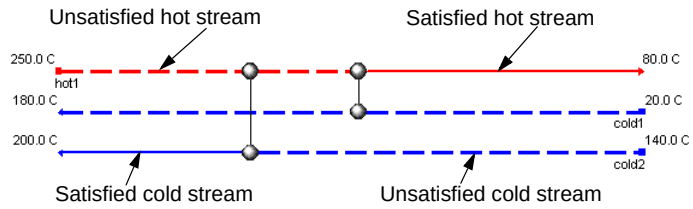
A typical Grid Diagram will contain four to five objects: process streams,

utility streams, heat exchangers, and splitters-mixers.

Streams

All process and utility streams in the heat exchanger network (HEN) system are displayed in the Grid Diagram. Initially, all process streams are shown “dashed” because their enthalpy is not satisfied. As the heat exchangers are placed in the streams, the streams become “solid”. With this feature, you can visually determine the unbalanced heating or cooling requirement for the streams.

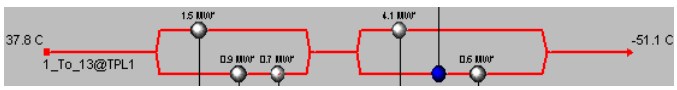
Figure 6.10



In **Figure 6.9**, the process streams are labelled: 1_to_13@TPL1, 22_to_24@TPL1, ToReboiler@COL1_to_ Boilerup@COL1, 81@COL1, and 82@COL1.

- The 1_to_13@TPL1 is a hot process stream as indicated by the red colour stream and the flow direction (from a high temperature to a low temperature).

Figure 6.11



- The other process streams are cold process streams as indicated by the blue colour stream and flow direction (from a low temperature to a high temperature).

Figure 6.12

The cold utility stream flow direction matches the flow direction of the cold process streams.

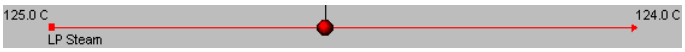
The cold utility stream is the blue arrow stream labelled Refrigerant 2.

Figure 6.13

The hot utility stream flow direction matches the flow direction of the hot process streams.

A hot utility stream called LP Steam is displayed in the figure below:

Figure 6.14



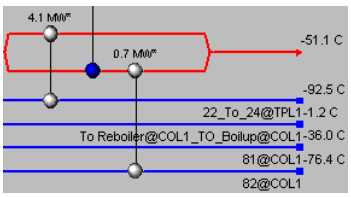
Heat Exchangers

The heat exchangers on the Grid Diagram appear as coloured disc laying on top of the stream flowing through it.

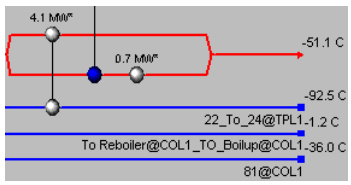
The heat exchanger in the Grid Diagram has two different appearances, depending on whether the stream attached to heat exchanger is visible or not.

- When the heat exchanger is attached to two streams that are visible/ displayed in the Grid Diagram, it will appear as coloured disc on each stream it is attached to, with a vertical line between the circles.

Figure 6.15



All streams displayed



82@COL1 stream has been hidden

The streams in the Grid Diagram can be hidden or displayed using the Property Presets option.

Refer to **Section 7.2.11 - Property Presets View** from the **Heat Integration** manual for more information.

- When one of the streams connected to the heat exchanger is not visible on the Grid Diagram, the heat exchanger will only appear as a coloured circle on the stream that is still visible.

There are five possible colours for the heat exchanger in the Grid Diagram. Each colour indicates a type of heat exchanger:

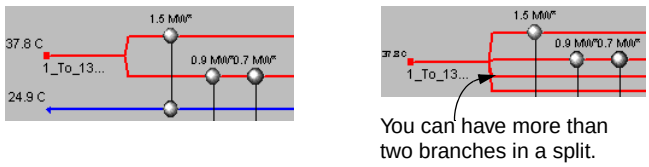
Color	Definition
Blue	Defines that heat exchanger as a cooler. In other words, the heat exchanger is attached to a hot process stream and a cold utility stream.
Red	Defines that heat exchanger as a heater. The heat exchanger is attached to a cold process stream and a hot utility stream.
Grey	Defines that heat exchanger as a process-process exchanger. The heat exchanger is attached to two process streams.
Yellow	Defines that heat exchanger is currently infeasible. Does not indicate if the exchanger is a cooler, heater, or process-process exchanger.
Green	Defines that the heat exchanger has been added/modified by a retrofit action.

Refer to **Section 5.5.2 - Modified Heat Exchangers** from the **Heat Integration manual** for more information.

Splitters and Mixers

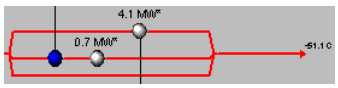
When a split occurs to a stream in the HEN, the split is indicated by the splitting/branching of a single arrow stream to a multiple arrow streams in the Grid Diagram.

Figure 6.16



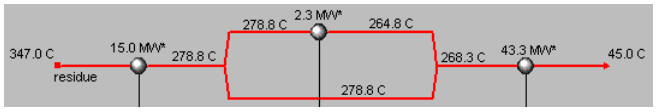
The splits/branches in the process stream will always converge back to a single arrow stream. The convergence of the branches indicates a mixer in the process stream.

Figure 6.17



The splitter-mixer option can be used to create by-passes.

Figure 6.18



The figure above is an example of a splitter-mixer added to the hot process stream to create a by-pass.

Refer to **Section 7.3.4 - Installing Splitters-Mixers** from the **Heat Integration** manual for more information about splitters and mixers in the Grid Diagram.

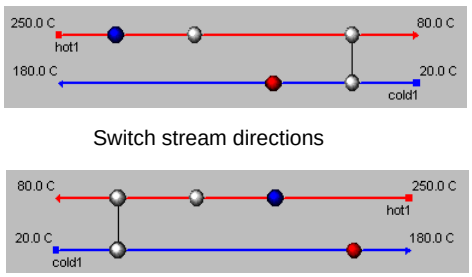
Customize Grid Diagram View

Refer to **Section 7.2.11 - Property Presets View** from the **Heat Integration** manual for more information on manipulating the Grid Diagram appearance.

HX-Net allows you to manipulate/modify the appearance of the HEN in the Grid Diagram. The Property Presets view contains the following options to modify the Grid Diagram:

- You can flip/switch the direction of the streams.

Figure 6.19



- You can display or hide the streams.
- You can rearrange the display order of the streams.
- You can display the three of the following information on the heat exchangers: load, area, HTC, name, or mean temperature difference.
- You can display the temperature and/or split fraction of the streams.

Cross Pinch Heat Load/Pinch Division

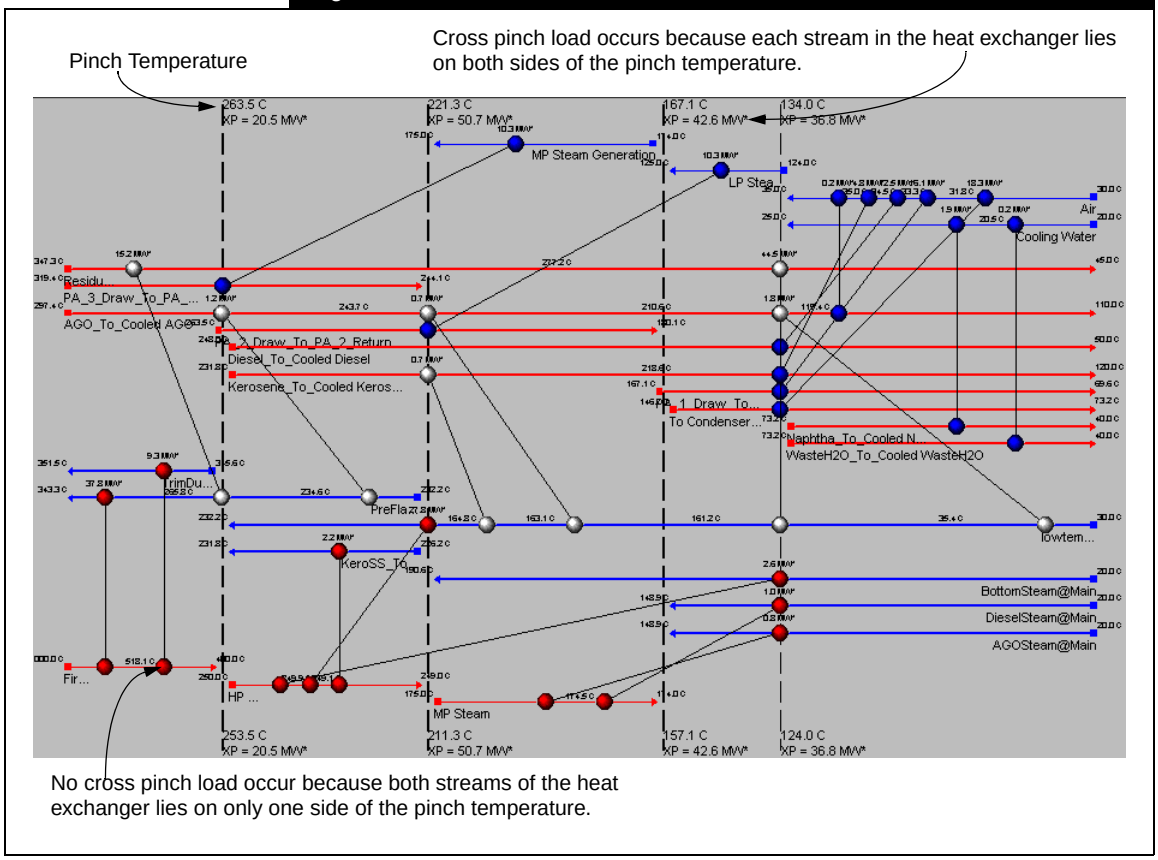
Refer to **Section 7.2.8 - Cross Pinch View** from the **Heat Integration** manual for more information about displaying the cross pinch load exchangers.

This program also identifies and displays heat exchangers that contain cross pinch heat load and the heat load values. A heat exchanger that has one of its streams' inlet and outlet temperatures lying on either side of the pinch temperature will have a *cross pinch load*.

The cross pinch load is the smaller of the two loads if the heat exchanger was calculated only to the pinch temperature from both the inlet and outlet temperatures.

The figure below is a Grid Diagram displaying cross pinch heat load and pinch temperatures.

Figure 6.20

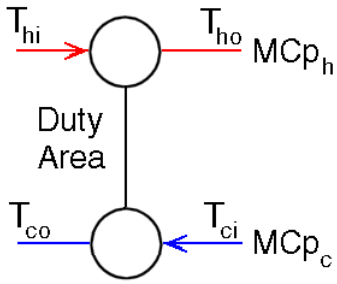


6.2.8 Degrees of Freedom Analysis

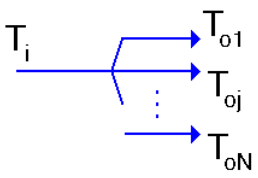
HX-Net determines the degrees of freedom for an entire network and not just for any specific unit operation.

The set equations used to determine the degrees of freedom in a network consists a combination of the following six equations depending on the layout of the network.

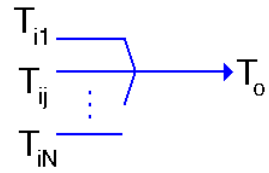
- **Equations (6.12)** to **(6.14)** are added to the equation set for each heat exchanger in the network.

Figure 6.21	Equations
	$Q = (T_{hi} - T_{ho}) \times MCp_h$ (6.12) $Q = (T_{ci} - T_{co}) \times MCp_c$ (6.13) $Q = U \times A \times \Delta T_{LM}$ (6.14) *where:* Q = *the total energy flow rate* A = *the heat transfer area* U = *the heat transfer coefficient* ΔT_{LM} = *the mean temperature difference*

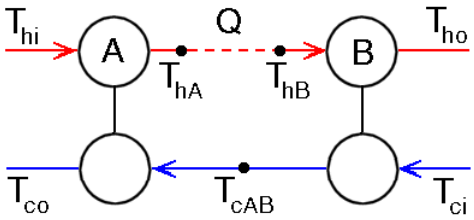
- For each splitter in the network **Equation (6.15)** is added.

Figure 6.22	Equation
	$T_{oj} = T_i$ for $j = 1,2,\ldots,N$ (6.15) *where:* N = *the number of branches*

- For each mixer in the network there is one **Equation (6.16)** which is added to the equation set.

Figure 6.23	Equation
	$\sum_{j=1}^{N} MCp_j \times T_{ij} = MCp_o \times T_o$ (6.16) *where: N = the number of branches*

- **Equation (6.17)** is used whenever there is a portion of a stream that is unsatisfied.

Figure 6.24	Equation
	$Q = MCp \times (T_{hA} - T_{hB})$ (6.17)

The above six equations make up the set of equations used in calculating the degrees of freedom. Degrees of freedom is the difference between the number of unknown variables and the number of equations. The possible unknown variables in the available equations are temperatures, duties, and area.

HX-Net uses the concept of nodes in determining the unknown variables. A node is a temperature point. Tying a stream reduces the number of equations that can be used because **Equation (6.17)** is not valid when two consecutive nodes are tied. A tied stream does not have an unsatisfied portion, or for that matter even the possibility of an unsatisfied portion. When a stream is tied there is only one temperature node between two heat exchangers.

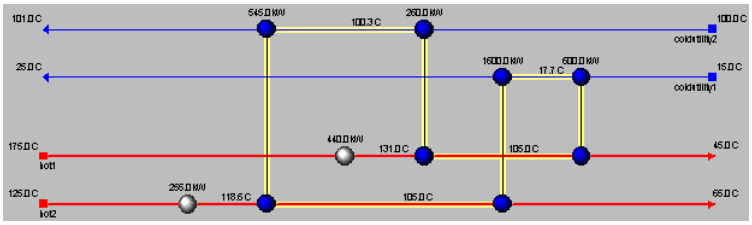
For example, **Figure 6.24** contains a cold stream that is tied and the hot stream is not. The resulting number of possible unknown variables is 11: Thi, ThA, ThB, Tho, Tco, TcAB, Tci, QA,QB, AreaA, and AreaB.

6.2.9 Loops in the Grid Diagram

The loop starts from an exchanger and flows along several exchangers and streams before ending back to the first exchanger. The heat exchangers in a loop does not have to be the same type.

A loop is a group of connection points consisting of exchangers that form a closed path in the Grid Diagram (Linnhoff et. al., 1982[89]). Refer to the figure below for an example of a loop:

Figure 6.25



A loop in the context of a PFD simulation is simply a recycle stream.

The presence of loops in a heat exchanger network (HEN) design may imply two statements:

- The HEN design has more heat exchangers than the minimum number required based on the Euler's General Network Theorem. The figure above shows that four coolers are being used to cool two hot streams, when perhaps two coolers would surfice.
- The HEN design has more constraints in its controllability.

Based on the possible occurrence of the previous two statements, when designing a HEN it is best to avoid loops whenever possible.

Loop Type

There are two types of loops in a heat exchanger network (HEN) design: independent and dependent.

HX-Net uses the following equation to determine the number of *independent loops* in a HEN design:

$$N_{loop} = (N_x - N_s) + N_n \quad (6.18)$$

where: N_{loop} = *the number of independent loops*

N_x = *the total number of heat exchanger units in the HEN design*

Only utility streams being used (connected to heat exchangers) are add to the total number of streams.

N_s = *the total number of streams (process and utility) in the HEN design*

N_n = *the total number of sub-networks in the HEN design*
A sub-network is a subset of the entire HEN design that has no interaction with the remaining heat exchanger network. Refer to ***Section 6.4.3 - Sub-networks*** *for more information about sub-network.*

Dependent loops represent all the loops available in the HEN design.

HX-Net uses the following steps to determine the number of *dependent loops* in a HEN design:

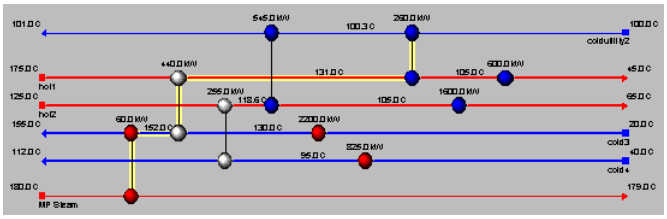
1. Start with a heat exchanger (A).
2. Follow a path from heat exchanger (A) to another heat exchanger (B).
3. Repeat the above step for the next heat exchanger until:
   - A path leads to the initial heat exchanger (A) again. This indicates that the path taken is a loop, and the stream-heat exchanger sequence encountered in path taken is stored.
   - A path that leads to just a stream with no other heat exchanger is encountered. This indicates that the path taken does not contain a loop.
4. Repeat steps #1 to #3 for all heat exchangers in the HEN design. Any repeated paths will be removed based on the stored stream-heat exchanger sequences.
5. When all the possible paths have been explored, HX-Net will have found all the possible loops in the HEN design.

6.2.10 Paths in the Grid Diagram

The path starts at a hot or cold utility stream and flows along exchangers and process streams before ending at a cold or hot utility stream.

A path is a group of connection points consisting of exchangers that form a path between a heater and a cooler in the Grid Diagram. Refer to the figure below for an example of a path:

Figure 6.26



The special characteristic about the path, is that a heat load can *shift* through it. An example is an increase in hot utility energy will reduce the heat transfer energy amount in an exchanger along the path. The change in energy transfer will also affect other heat exchangers along the path. So the heat load is being *shifted* from exchanger to exchanger, until the cooler. The cooler at the end of the path will need to reduced the energy that was added into the hot utility.

Both loops and paths can be manipulated to reduce the cost and increase the efficiency of an HEN design. HX-Net recommend using the following two steps to manipulate both paths and loops, and reduce the number of heat exchangers in the HEN design.

1. Break the loop containing the exchanger with the smallest heat load, by removing the exchanger.
2. Relax the paths by shifting the heat load, so the minimum temperature difference between streams in heat exchangers are restored.

6.2.11 Forbidden Matches

For information on how to specify forbidden matches, refer to **Section 1.5 - Forbidden Matches View** from the **Heat Integration** manual.

In some situations, two process streams cannot be allowed to exchange heat with one another. This can be due to considerations like plant layout, corrosion, or available material for construction. Such constrained matching considerations are called Forbidden Matches.

6.3 Targets

Targets are theoretical values that represent the ideal or perfect situation. They are very important as an analysis tool as it provides a comparison for how close the current design is to the optimal design.

6.3.1 Energy Targets

For more information on Utility Load Allocation Methods, refer to **Section 6.3.2 - Utility Load Allocation Methods**.

Energy targets are the minimum amount of utilities needed to satisfy the process stream requirements (Papoulias & Grossmann, 1983[106] and Cerda & Westerberg, 1983[23]). In HX-Net, the energy target values are calculated depending on the *Utility Load Allocation Method* and pinch temperature. The hot and cold utility energy targets are both displayed.

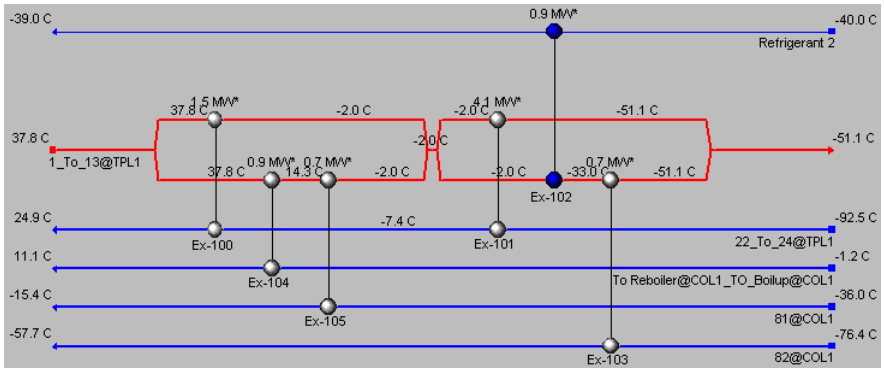
Pinch Temperature

The pinch temperature is used in designing the optimal HEN by identifying the following:

- Impossible heat transfer between streams when the temperature difference between streams is equal or less than the pinch temperature.
- Unnecessary use of cold utility, when a cold utility is used to cool hot streams in the region above the pinch.
- Unnecessary use of hot utility, when a hot utility is used to heat cold streams in the region below the pinch.

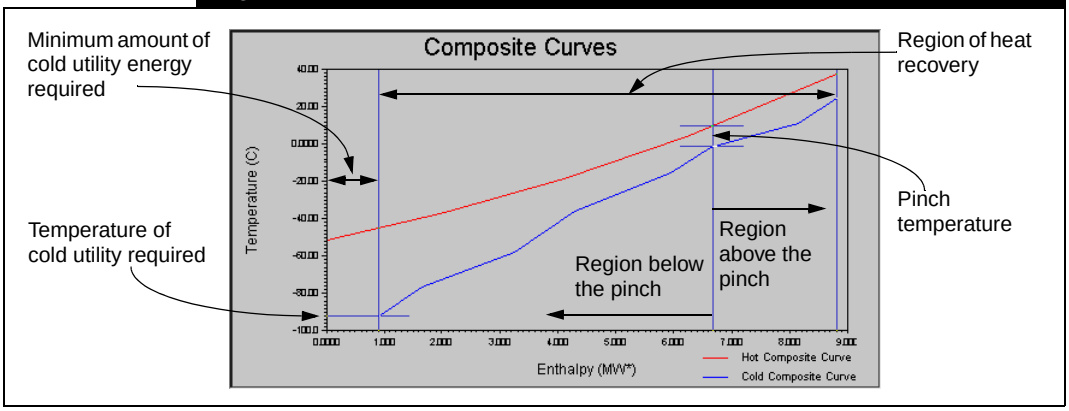
For example, consider the following heat exchanger network (HEN) design:

Figure 6.27



Based on the HEN design, the following Composite Curves graph is formed:

Figure 6.28



The above graph plots the temperature and energy transfer required from all the process streams from the HEN.

From the graph, you can clearly identify:

- The minimum cold utility required and at what temperature does the cold utility have to be.
- The pinch temperature of the HEN, which indicates the minimum temperature difference between streams.

- The possible region of heat recovery by using process-process heat exchangers.
  Process-process heat exchangers are exchangers that uses the hot process streams in the HEN to heat the cold process streams in the HEN and vice versa. So amount of external (utility) energy required to heat or cool the process streams is reduced.

The pinch temperatures occur at:

- the minimum temperature difference between hot stream and cold stream temperature when both hot and cold stream have the same heat flow.
- the temperature when the net heat flows in the process is zero.

There are two pinch types:

- **Process Pinch**. Divides the process into two parts: A high temperature region above pinch which accepts hot utilities and a lower temperature region below pinch which accepts cold utilities. At a particular minimum approach temperature, the pinch occurs where the hot and cold composite curves are ΔT_{min} apart.
- **Utility Pinch**. Created whenever a utility stream curve touches the grand composite curve. Utility pinches can be observed in a shifted balanced composite curves. Like the process pinch, the hot and cold composite curves are ΔT_{min} apart at utility pinches.

6.3.2 Utility Load Allocation Methods

A problem arises when you have more than one hot and/or cold utility. You must determine the optimum usage levels of the available utilities which will minimize operating costs, and satisfy the overall utility target requirements.

GCC Based Method

The *GCC Based Method* uses the Grand Composite Curve to allocate utilities (Linnhoff et. al. 1982[89], Parker 1989[107]). The general heuristic is to maximize the use of the cheapest utilities. This is based on the assumption that the least expensive utilities are the hottest cold utilities and the coldest hot utilities.

In this program, a utility is considered cheap not based on cost but based on temperature. A hot utility at a lower temperature is cheaper than a hot utility at a higher temperature.

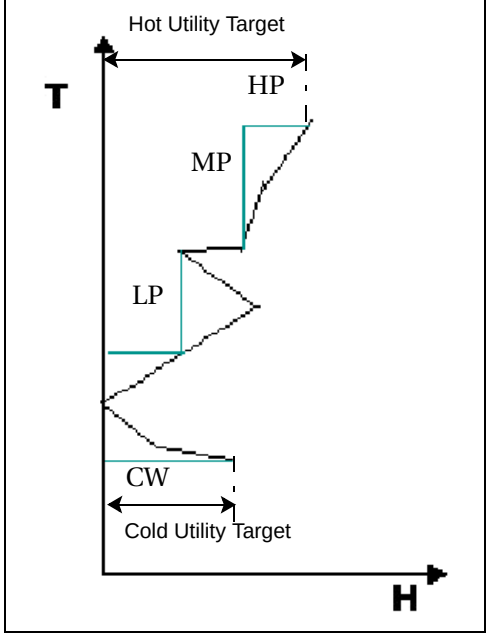
The following methodology is used to allocate utilities using the GCC Based Method:

The Grand Composite curve is a plot of shifted temperatures versus the cascaded heat between each temperature interval.

From the GCC, you can determine the minimum hot and cold utility requirements for the network.

1. Generate the Grand Composite Curve associated with the hot and cold process streams.

Figure 6.29



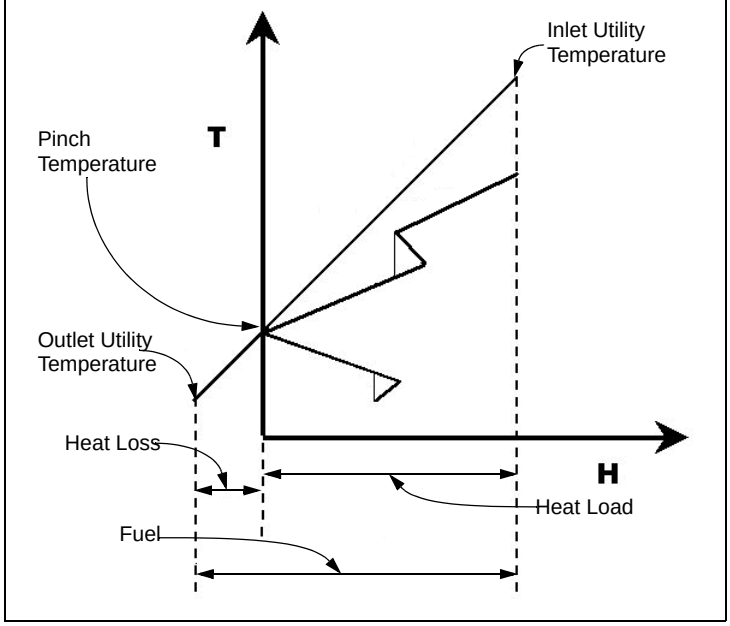
2. Since the Grand Composite Curve is plotted in terms of shifted temperatures, you are required to shift the utility temperatures. The hot utility temperatures must be decreased by $\Delta T_{min}/2$ and the cold utility temperatures must be increased by $\Delta T_{min}/2$.
3. Isolate all pockets in the GCC. It is assumed that pockets are self-sufficient in energy.

For point utilities see steps #4 to #7. For non-point utilities see steps #8 to #10.

4. It is assumed that the utilities closest to the pinch are the least expensive. For hot utility streams, use the utility with the lowest outlet temperature first. For cold utility streams, use the utility with the highest outlet temperature first.
5. Draw the first (least expensive) utility line from the temperature axis to the Grand Composite curve. Do not extend the utility line beyond the entrance of any pockets in the GCC.

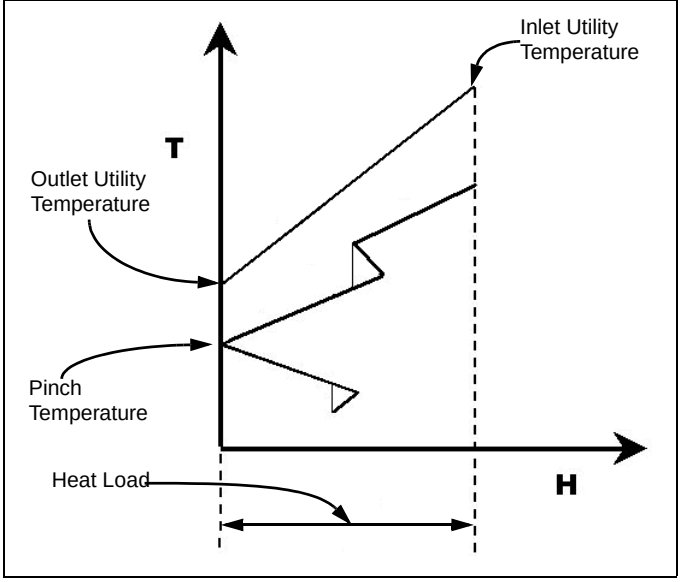
6. Draw a vertical line from the outlet temperature of the first utility line to the inlet temperature of the next (second least expensive) utility.
7. Continue using utility streams in this manner until you satisfy the minimum required utility load (target utility load).
8. Plot the inlet utility temperature vertically above the end vertex of the Grand Composite Curve.
9. Depending on the outlet utility temperature, pinch temperature, and the shape of the GCC, there are three possibilities.
   - If the outlet utility temperature is below the pinch temperature, draw a line from the inlet utility temperature to the pinch point. Extend this line to the outlet utility temperature. The load and losses can be determined graphically as shown below.

Figure 6.30



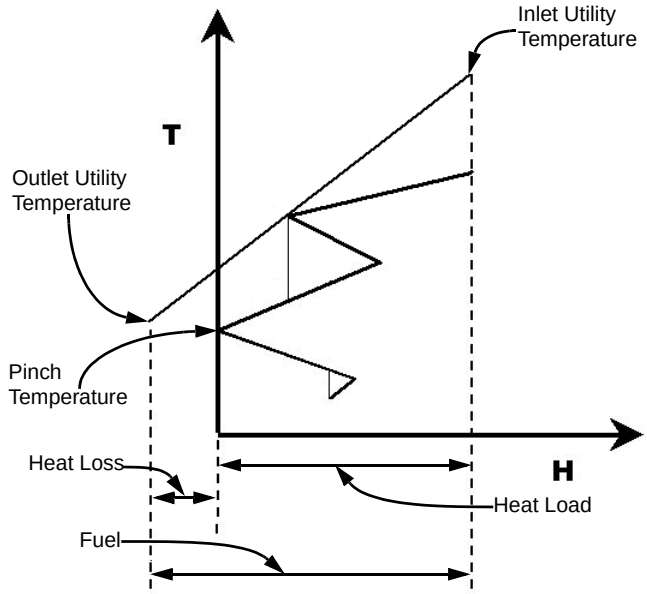
- If the outlet utility temperature is greater than the pinch temperature, draw a line from the inlet utility temperature to the outlet utility temperature on the temperature axis.

Figure 6.31



- If a large pocket exists in the GCC and is situated between the inlet and outlet utility temperatures, draw a line from the outlet pinch temperature to the inlet temperature such that it touches the GCC only at one point. The load and losses can be determined graphically as shown below.

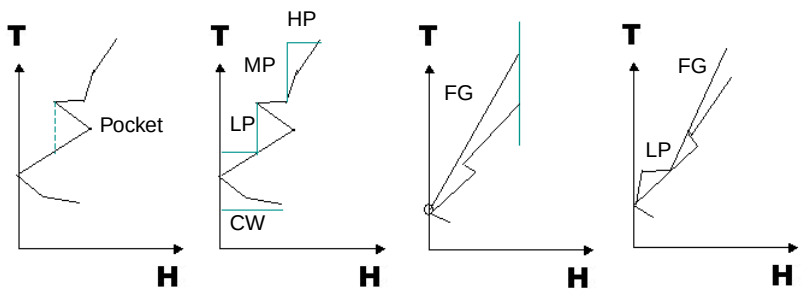
Figure 6.32



10. Continue using other utility streams in this manner if the minimum required utility load (target utility load) is not satisfied.

The figure below demonstrates how different utilities are allocated using the GCC Based method.

Figure 6.33



By following the GCC Method, you maximize the use of the hottest cold utilities and the coldest hot utilities in the process.

User Supplied Utility Loads Method

This method is not available if there are forbidden matches in the heat exchanger network (HEN).

If the *User Supplied Utility Loads* method is selected, you can allocate individual utility loads in the HEN. Using this method, you can modify the *Heat Load*.

However, you cannot specify unreasonable heat loads for any utility. All heat utility allocations must be thermodynamically feasible in order to be accepted by this program. You must allocate hot and cold utilities such that the difference between the hot and cold utility loads is always equal to the difference between the hot and cold utility targets.

Keep in mind that hot utilities crossing the pinch will result with heat loses.

A warning message will appear if you attempt to model impossible utility allocations in HX-Net.

Cheapest Utility Principle (CUP)

This method is not available if there are forbidden matches in the heat exchanger network (HEN).

This method is best used when there is a linear relationship between the total exchanger area and the total capital cost.

The CUP method is use to decide which utilities to implement in a heat exchanger network (HEN) that would be cost effective. This method takes into account the capital investment as well as the energy cost while calculating targets for the utility load (Shenoy et. al., 1998[138]).

The significance of this targeting approach in the design of the HEN is two fold:

- The HEN generated based on these targets is near-optimal.
- The HEN can be generated using the conventional pinch design method and very little evolution is necessary, saving the designer time and money.

CUP states that the increase in the load of the cheapest utility increases the total utility consumption while maintaining the load of the relatively higher cost utilities constant (Shenoy 1998[137]). The driving forces at the utility pinches do not vary with the minimum approach temperature.

The Cheapest Utility Principle option requires both cold and hot utility streams to meet utility requirements. Otherwise, both utility stream status bars will be displayed as Insufficient.

6.3.3 Area Targets

The area targets are the minimum amount of heat transfer area required for the hot and cold streams in a heat exchanger network (HEN) to achieve their specified temperature values.

This equation is also known as the *Uniform BATH Formula*, for more information refer to the **Vertical Matching (Bath Formula)** section.

The basic equation used to calculate the area target is:

$$A = \sum_i \left(\frac{1}{F_t \times \Delta T_{LM}} \right)_i \times \sum_j \left[(dT_h)_i \times \sum_{jh} \left(\frac{MC_p}{h} \right)_{jh} + (dT_c)_i \times \sum_{jc} \left(\frac{MC_p}{c} \right)_{jc} \right] \quad (6.19)$$

where: A = *the target area*

The F_t is 1 for a counter current exchangers, and less than 1 for other configurations.

F_t = *the correction factor accounting for non-counter current flow*

ΔT_{LM} = *the logarithmic mean temperature difference at each interval*

i = *denotes the i-th enthalpy interval*

j = *denotes the j-th stream*

dT_h = *the temperature change for the hot stream at each enthalpy interval*

M = *the mass flow rate of the stream*

C_p = *the specific heat capacity of the stream*

This h value may vary, depending on the type of exchanger.

h = *the heat transfer of the stream*

dT_c = *the temperature change for the cold stream at each enthalpy interval*

The area targets are used in the calculation of the total capital cost of the heat exchangers.

HX-Net calculates and provides two different area targets:

- *Counter Current area*. Assuming all heat exchangers in the HEN are counter-current type.
- *1-2 Shell & Tube area*. Assuming all heat exchangers in the HEN are 1-2 shell and tube type.

There are two different methods used to calculate the area targets: Bath Formula and LP Formulation.

When you specify a forbidden match, the area target method will automatically switch from the *Bath Formula* to *LP formulation*. Similarly, the utility allocation method (refer to **Section 6.3.2 - Utility Load Allocation Methods**) changes to *GCC Based*. Targets will be recalculated based on the specified forbidden matches.

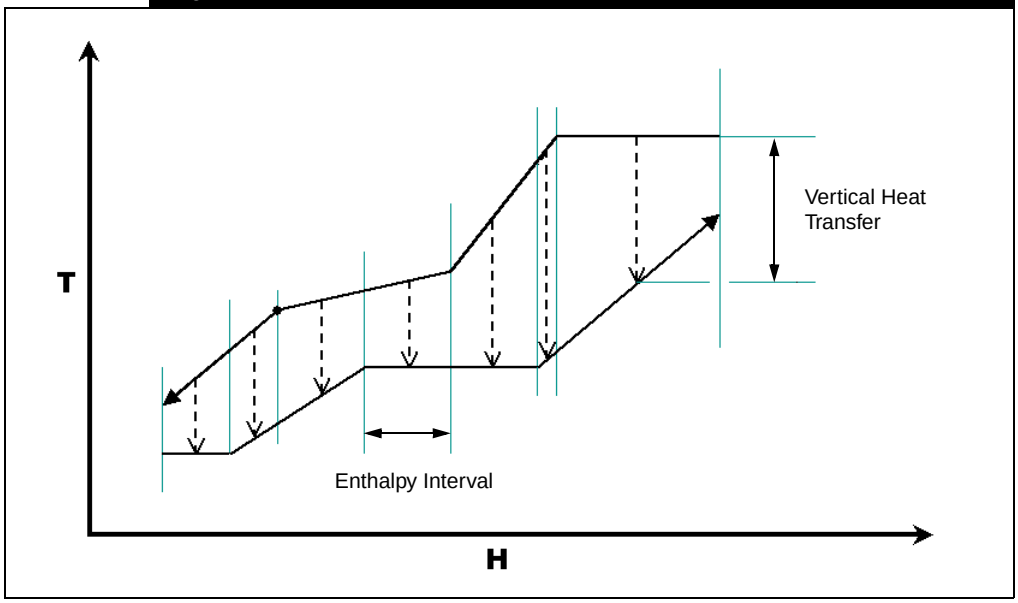
Vertical Matching (Bath Formula)

The area target using the *Bath Formula* is calculated with the assumption that only countercurrent heat exchange exists between the hot and cold process streams (Townsend & Linnhoff, 1984[151]).

Only “vertical” heat transfer occurs between the hot and cold streams in the composite curves. That is, heat exchanger matches can only occur within the same enthalpy interval on the composite curves.

The figure below shows examples of “vertical” heat transfer.

Figure 6.34



The area target calculated by the Bath Formula provides minimum area if the local heat transfer coefficients are similar in value.

For each heat exchanger in an interval, the area is calculated as follows:

$$A_{er} = \frac{Q_{ijek}}{\Delta T_{LM}}\left(\frac{1}{h_{i,h}} + \frac{1}{h_{i,c}}\right) \qquad (6.20)$$

where: A = *the target area*

Q = *the total amount of energy transferred*

ΔT_{LM} = *the logarithmic mean temperature difference*

h = *the heat transfer of the stream at each interval*

$_{h,c}$ = *denotes the hot or cold streams respectively*

You can calculate the area target of the heat exchanger network by summing all heat exchanger areas for each interval in the network.

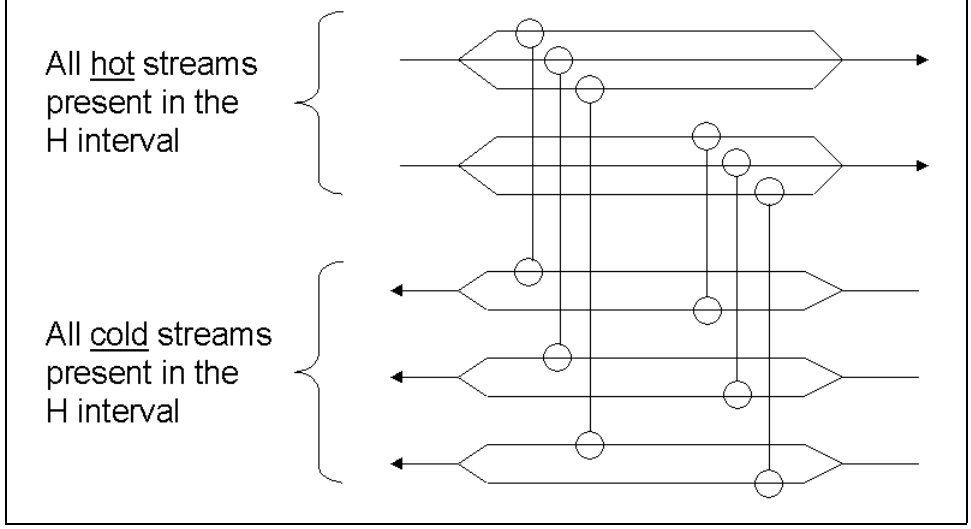
$$A_{network} = \sum_{k=1}^{n \text{ interval}} \frac{1}{\Delta T_{LM,k}} \left(\sum_{i}^{\text{hot streams}} \frac{q_i}{h_i} + \sum_{i}^{\text{cold streams}} \frac{q_i}{h_i} \right) \quad (6.21)$$

where: q = the amount of energy transferred at each interval

The **Equation (6.21)** is known as the Bath Formula. This equation assumes that a spaghetti Network exists between each enthalpy interval shown in the following figure.

In a Spaghetti network, every hot stream exchanges heat with every cold stream present in the interval.

Figure 6.35



This calculation method is used by default in HX-Net, but will not be used when forbidden matches occur in the system.

LP Formulation

A more complex area targeting calculation method is the *LP* (Linear Programming) *Formulation* (Cerda et. al., 1983[22], Papoulias & Grossmann, 1983[106], and Shethna et. al., 2002[141]). This method is not restricted, like the Vertical Matching method, to vertical heat transfer.

If the local heat transfer coefficients do not vary widely, the area targets predicted by the Bath Formula should be adequate in most cases.

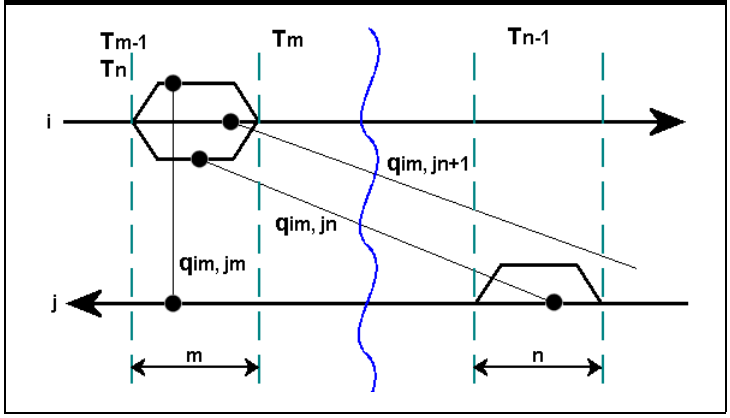
The heat transfer matches can cross the enthalpy intervals in the composite curves. If the local heat transfer coefficients are different enough, crisscrossed heat exchange can result in lower predicted area targets. However, it has been shown that the minimum area predicted by the LP Formulation will not deviate more than 10% from that predicted by the Bath Formula, even when the heat transfer coefficients differ by one order of magnitude.

You can specify forbidden matches between streams using the LP Formulation. HX-Net uses a linear optimization model to minimize the area target. The LP Formulation first matches all thermodynamically feasible streams in the heat exchanger. It then performs an optimization on the following equation:

$$Minimize\ A_{network} = \sum_{k} \frac{Q_k}{U_k \Delta T_{LM,k}} \tag{6.22}$$

The following figure and equations illustrate how the LP Formulation matches thermodynamically feasible streams to obtain the ΔT_{LM} for each interval:

Figure 6.36



The temperature in a match between a stream *i* in interval *m*, and a stream *j* in interval *n* are the same as the temperature in interval *m* and *n*. With these known temperatures the following equations are used to determine the ΔT_{LM}.

$$\Delta T^{H}_{im,jn} \equiv \Delta T^{H}_{m,n} = T_{m-1} - T_{n-1}$$
$$\Delta T^{C}_{im,jn} \equiv \Delta T^{C}_{m,n} = T_{m} - T_{n} \qquad (6.23)$$
$$i \in H_m, j \in C_n, m,n \in K$$

$$(\Delta T_{LM})_{im,jn} \equiv (\Delta T_{LM})_{m,n} \qquad (6.24)$$

where: ΔT = *the temperature approach at match*

H = *the hot stream*

C = *the cold stream*

K = *the number of intervals*

ΔT_{LM} = *the logarithmic mean temperature difference*

The number of temperature intervals for the calculation is determined using the following procedure:

1. Part of the number of intervals in a stream is determined by the number of segments in the stream (based on different enthalpies due to temperature changes).
2. The following two formulas are used to determine the second part of the number of intervals:

$$N_{add} = ceil[dT_k / dT_{mean}]$$
$$dT_{mean} = max[3 \times dT^{min}, 10] \quad (6.25)$$

where: N_{add} *= the number of intervals based on the smallest temperature interval size*

$ceil[x]$ *= the nearest integer number not less than x*

dT^{min} *= the smallest temperature interval size from the first step in obtaining the number of intervals for the calculation*

dT_k *= the temperature at interval i*
The interval k is the interval obtained from the first step.

The final amount of intervals is the sum of the intervals from step #1 and #2. The final number of intervals will give accurate results within a reasonable amount of computation time.

In HX-Net, this calculation is used only when there is at least one forbidden match present between streams.

6.3.4 Number of Units Targets

Unit and shell targeting involve the calculation of the minimum number of units and shells in the heat exchanger network. The calculation is based on Euler's Network Theorem (Linnoff et. al., 1982[89] and Ahmad et. al., 1990[6]).

$$N_{u,\,min} = N_s + N_l - N_i \tag{6.26}$$

where: $N_{u,min}$ = *the unit target*

N_s = *the number of process and utility streams*

N_l = *the number of heat exchanger loops*

N_i = *the number of independent systems*

Equation (6.26) is the minimum number of units in the heat exchanger network, not considering the existence of the pinch.

A subset is an independent set of streams that exchange heat with one another. The streams contained within a subset are in heat balance and are thermodynamically compatible.

The primary reason for calculating subsets is to simplify networks with a large number of streams. The complexity of a large network of streams decreases significantly if it is divided into a number of smaller independent subsets. In addition, creating subsets in a heat exchanger network increases the number of independent systems and hence reduces the minimum number of units.

Subsets are calculated using the following procedure (Shethna et. al., 1998[139]):

1. Calculate all possible and thermodynamically feasible subsets that do not include utility streams.
2. Calculate all possible and thermodynamically feasible subsets with remaining and utility streams.

The minimum overall unit target can be expressed as:

$$N_{u,\,min} = N_s - 1 \tag{6.27}$$

where: $N_{u,min}$ = *the unit target*

N_s = *the number of process and utility streams*

Equation (6.27) is the minimum number of units in the heat exchanger network, not considering the existence of the pinch.

In order to consider maximum energy recovery in the calculation of the minimum number of units in the heat exchanger network, the existence of the pinch must be considered.

The minimum number of units considering the pinch is calculated as follows:

$$N_{u,\,min} = (N_A - 1) + (N_B - 1) \tag{6.28}$$

where: $N_{u,min}$ = *the unit target*

N_A = *the number of process and utility streams above the pinch*

N_B = *the number of process and utility streams below the pinch*

Shell Targeting involves the calculation of the minimum number of shells in the heat exchanger network. A heat exchanger unit can need more than one shell depending on the configuration of the heat exchanger or restriction on the shell area.

6.3.5 Cost Targets

For more information on capital cost, operating cost, and TAC, refer **Section 6.2.6 - Economic Parameters**.

The *total annual cost* of a heat exchanger network (HEN) is comprised of two parts: the capital cost and the operating cost.

- The **operating cost** network is the cost required to operate the process ($/yr).
- The **capital cost** of the network is a single investment required to build the heat exchanger network ($).

The target capital cost depends largely on how the area targets were calculated and what heat exchanger configurations are used in the HEN design.

In calculating the target capital cost the following assumptions are used in the calculation:

- The following values are used in the calculation: the minimum number of shells, the required number of exchangers to achieve maximum energy recovery, and the area target value from an exchanger.
- The heat exchanger area is distributed evenly among all the heat exchangers.
- All heat exchangers use the same cost law/set coefficients.

In actual plants, the capital cost of exchangers with different service conditions can vary widely across the heat exchanger network. Assuming uniform exchanger specifications can result in unreasonable area targets.

For more information on Matchwise Economics, refer to **Section 1.4 - Matchwise Economic View** from the **Heat Integration** manual.

The individual capital cost of heat exchangers in a HEN can be calculated by specifying different cost sets for specific hot and cold stream pairs.

6.3.6 Range Targeting

Range Targeting contains information pertinent to the optimization of the minimum approach temperature, ΔT_{min}. Traditionally, the ΔT_{min} used in designing heat exchanger networks is determined using experience and heuristic methods.

An optimum minimum approach temperature is calculated by minimizing the total annual cost (Ahmad & Linnhoff, 1989[4] and Ahmad et. al., 1990[6]). This means finding the best compromise between utility requirements, heat exchanger area and unit and shell number. As the minimum approach temperature is varied the total annual cost of the network is calculated. There will be a ΔT_{min} which will yield a minimum total annual cost.

For more information on TAC, refer to the **Total Annualized Cost** section in **Section 6.2.6 - Economic Parameters**.

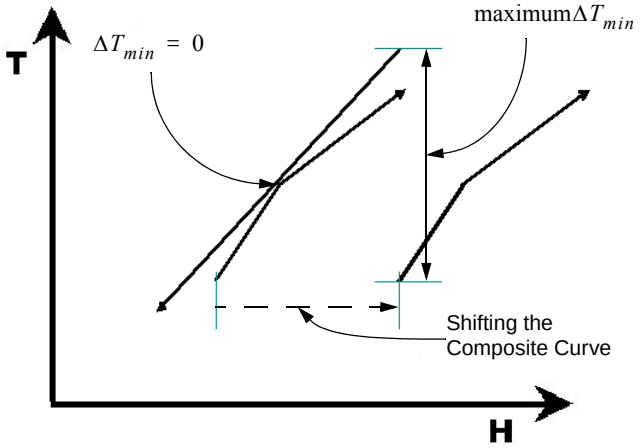
The total annual cost (TAC) of the heat exchanger network is the sum of the total operating and capital costs.

It can be observed from the hot and cold composite curves that an *increase* in the minimum approach temperature *increases* the total operating costs of a heat exchanger network. Increasing the minimum approach temperature horizontally shifts the composite curves away from one another. Consequently, the minimum utility requirements (utility targets) increase.

Unlike operating costs, an *increase* in the minimum approach temperature *decreases* the total associated capital of a heat exchanger network. Because the composite curves are further apart, there is a higher temperature driving force. As a result, less area is required for the same amount of heat transfer.

The minimum approach temperature, ΔT_{min}, can range from 0 to a maximum value. The maximum ΔT_{min} results when the composite curves are situated such that there is no heat integration between the hot and cold process streams.

Figure 6.37



The general procedure used in HX-Net to determine an optimum minimum approach temperature for a heat exchanger network is as follows:

1. Determine the maximum and minimum ΔT_{min}, using the hot and cold composite curves.
2. Start with the minimum ΔT_{min} and determine the utility, area, and unit and shell targets.
3. Determine the TAC from the capital cost target and the operating cost target.
4. Repeat steps #2 and #3 using various values of ΔT_{min}. The ΔT_{min} intervals are determined using the Golden Search method.
5. Plot the TAC with the ΔT_{min}. The minimum TAC corresponds with the optimum ΔT_{min}.

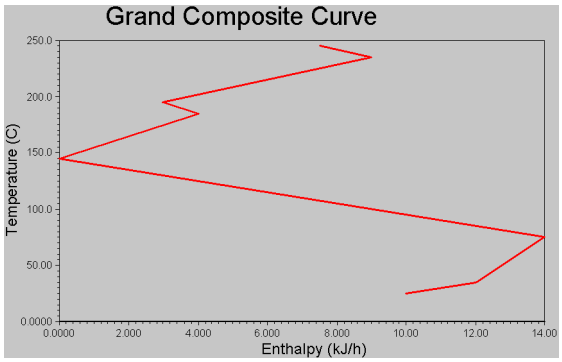
6.3.7 Plots

Plots provide a visual analysis of key variables and trends for the heat integration in a given stream data. HX-Net has a wide variety of plots available.

Grand Composite Curve

The Grand Composite Curve is a plot of shifted temperatures versus the cascaded heat between each temperature interval (Linnhoff et. al. 1982[89]). It shows the heat available in various temperature intervals and the net heat flow in the process (which is zero at the pinch). A grand composite curve sample is displayed in the figure below.

Figure 6.38

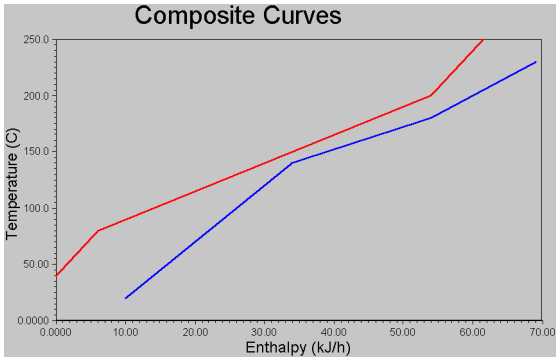


Composite Curve

A Composite Curve is a graphical combination (or composite) of all hot or cold process streams in a heat exchange network (Linnhoff et. al. 1982[89]). The Composite Curve plot displays both the hot composite curve and cold composite curve on the same plot. The closest temperature difference between the hot and cold composite curves is know as the minimum approach temperature, ΔT_{min}.

The composite curves are moved horizontally such that the minimum approach temperature on the plot equals the minimum approach temperature you specified.

Figure 6.39



Shifted Composite Curve

The Shifted Composite Curve is constructed the same way as the Composite Curve (Linnhoff et. al. 1982[89]). However, the Hot Composite Curve (HCC) is shifted down by $\Delta T_{min}/2$ and the Cold Composite Curve (CCC) is shifted up by $\Delta T_{min}/2$. The following equations show how the shifted temperatures are calculated:

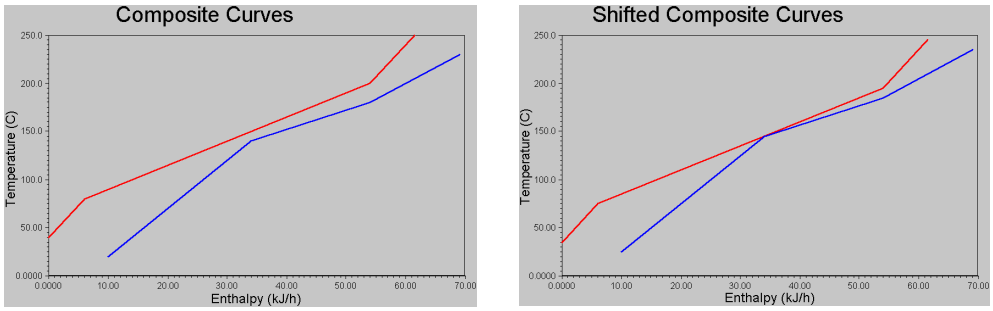
$$\text{Shifted Hot Stream Temperature} = \text{Unshifted Hot Stream Temperature} - \Delta T_{min}/2 \quad (6.29)$$

$$\text{Shifted Cold Stream Temperature} = \text{Unshifted Cold Stream Temperature} + \Delta T_{min}/2 \quad (6.30)$$

The result is that the hot and cold composite curves meet at the pinch location.

The figure below displays the unshifted and shifted composite curves. It can be observed that the two curves are shifted vertically.

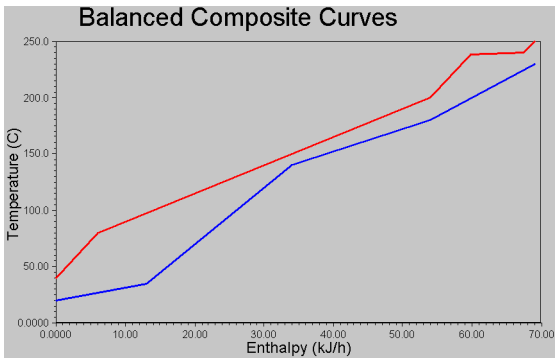
Figure 6.40



Balanced Composite Curve

The Balanced Composite Curve is constructed the same way as the Composite Curve (Linnhoff et. al. 1982[89]). However, the Balanced Composite Curve is a combination of both the utility and process streams. The HCC is a composite of both the hot process and utility streams. The CCC is a composite of both the cold process and utility streams.

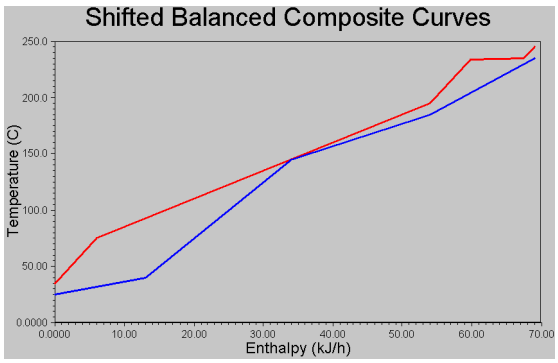
Figure 6.41



Shifted Balanced Composite Curve

The Shifted Balanced Composite Curve is constructed the same way as the Shifted Composite Curve (Linnhoff et. al. 1982[89]). However, the Shifted Balanced Composite Curve is a combination of both the utility and process streams. The Shifted HCC is a composite of both the hot process and utility streams. The Shifted CCC is a composite of both the cold process and utility streams The HCC and CCC touch each other at the pinch points on this curve.

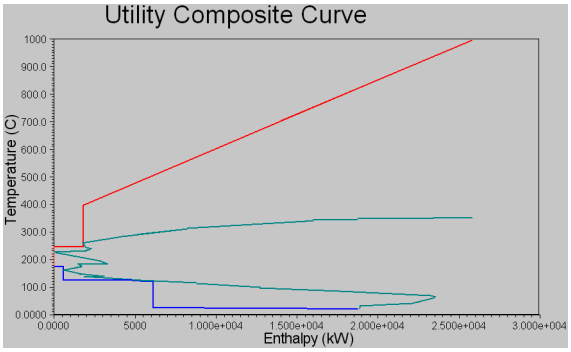
Figure 6.42



Utility Composite Curve

The Utility Composite Curve is constructed much like a GCC (Linnhoff et. al. 1982[89]). However, in addition to the GCC, the Utility Composite Curve contains hot and cold utility streams. From the Utility Composite Curve plot, you can determine the minimum hot and cold utility requirements for the network as well as visually inspect how much of each utility contributes to the total utility target.

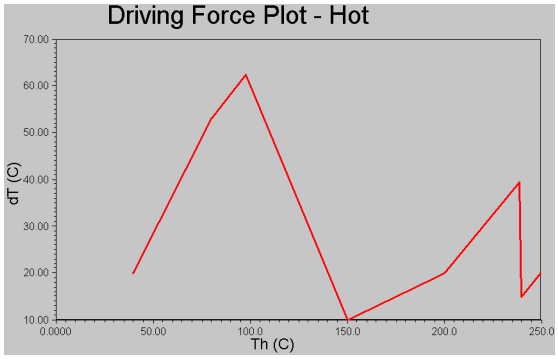
Figure 6.43



Hot Driving Force Curve

The Hot Driving Force Curve plots the temperature difference (driving force) between the hot and cold composite curves (Linnhoff 1993[97]). The temperature difference between the two composite curves are plotted against the hot stream temperature. It depicts how driving forces vary with hot temperatures.

Figure 6.44

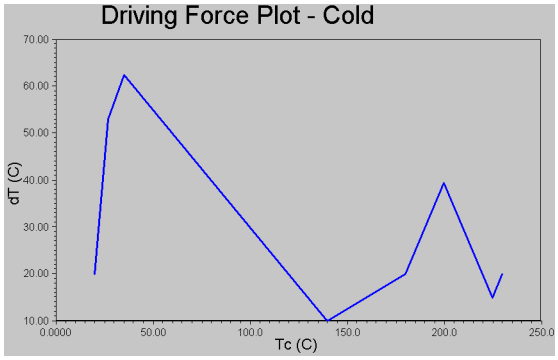


The pinch of the heat exchanger network can be observed as the lowest point of the curve, closest to the X axis.

Cold Driving Force Curve

The Cold Driving Force Curve plots the temperature difference (driving force) between the hot and cold composite curves (Linnhoff 1993[97]). The temperature difference between the two composite curves are plotted against the cold stream temperature. It depicts how driving forces vary with cold temperatures.

Figure 6.45



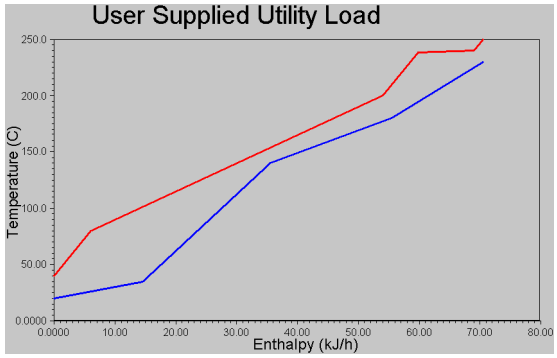
The pinch of the heat exchanger network can be observed as the lowest point of the curve, closest to the X axis.

User Supplied Utility Load Plot

For more information on the User Supplied Utility Loads, refer to **Section 6.3.2 - Utility Load Allocation Methods**.

The User Supplied Utility Load Curve is essentially a composite curve of the utility streams specified by the user.

Figure 6.46



6.4 Controllability

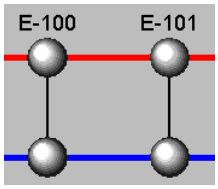
For information on accessing the controllability status of the HEN, refer to **Section 7.9 - Topology View** from the **Heat Integration** manual.

In a heat exchanger network (HEN) design, the variables you want to control are the process stream's outlet temperatures. If you control the output temperatures, than you do not have to worry about the possibility of temperature fluctuation from the process streams effecting the rest of your process.

To be able to control the output temperature of the streams in the HEN design, you have to check if the HEN design has enough manipulated variables/degrees of freedom to implement controls on to the design.

6.4.1 Manipulated Variables

Usually the number of manipulated variables in the HEN design equals the total number of heat exchangers in the design. However if there are loops in the design, each loop reduce the number of manipulated variables by one.



Notice the two heat exchangers forms a loop in the HEN design.

For example, take two process streams using two heat exchangers to perform the necessary heat transfer between each other. You may assume since there are two heat exchangers that means there are two manipulated variables. However, both heat exchangers are on the same two process streams, changing the heating duty (manipulating) one of the heat exchanger will automatically affect the other heat exchanger. Since you cannot manipulate one without affecting the other, you really only have one manipulated variable.

The number of manipulated variables is calculated using the following equation:

$$N_{mv} = N_x - N_{loop} \tag{6.31}$$

where: N_{mv} = *the number of manipulated variables*

N_x = *the total number of heat exchanger units in the HEN design*

Refer to **Section 6.2.9 - Loops in the Grid Diagram** for information about loops.

N_{loop} = *the number of loops in the HEN design*
The number of loops only consist of loops without utility exchangers, because loops containing the utility exchangers are assumed to be able to handle any upsets/changes in temperature.

6.4.2 Degrees of Freedom

The value of the degrees of freedom indicates whether the HEN design can be controlled or not:

- $N_{DoF} < 0$ indicates that there is not enough manipulated variables in the HEN design and it is not possible to control all target temperatures.
- $N_{DoF} = 0$ indicates that there is enough manipulated variables in the HEN design to control the target streams' temperatures.
- $N_{DoF} > 0$ indicates that there is enough manipulated variables in the HEN design and you can implement more sophisticate control structures.

The number of degrees of freedom is calculated using the following equation:

$$N_{DoF} = N_{mv} - N_{ts} \tag{6.32}$$

where: N_{DoF} = *the number of degrees of freedom*

N_{ts} = *the number of target streams*

Target streams are process streams whose output temperature is controlled.

For example, consider two streams: one entering a storage tank and another entering a reactor. The temperature of a stream entering a storage tank need not have a fixed temperature, so it is not a target stream. The temperature of a stream entering a reactor tank requires to be at a specific value for the reaction to occur, so the stream is a target stream.

6.4.3 Sub-networks

The sub-networks in a HEN design is another factor that affects the controllability status of the design.

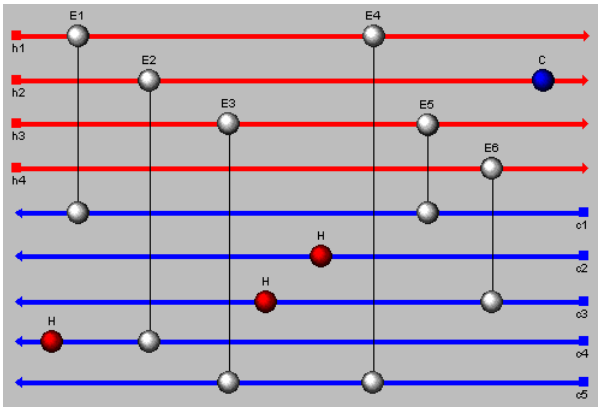
A sub-network in the Grid Diagram is a set of streams that are heated and/or cooled within the set and does not affect other streams in the entire heat exchanger network (HEN).

Calculating Degrees of Freedom

When calculating the degrees of freedom, you may generate a result of **0** when considering the entire HEN design. However, if you consider calculating the degrees of freedom for each sub-network in the HEN design, the sub-network degrees of freedom values may not be the same as the degrees of freedom value for the entire HEN design.

For example, consider the HEN design in the figure below, where all target temperatures should be controlled:

Figure 6.47



The number of degrees of freedom for the entire HEN design is $N_{DoF} = 10 - 1 - 9 = 0$. The degrees of freedom value seem to indicate that the HEN design can be controlled and there is sufficient manipulated variables.

Now consider the four sub-networks in the HEN design:

- Sub-network 1 consist of **h1**, **h3**, **c1**, **c5**, **E1**, **E3**, **E4**, and **E5**. The degrees of freedom is $N_{DoF} = 4 - 1 - 4 = -1$.
- Sub-network 2 consist of **h4**, **c3**, **H**, and **E6**. The degrees of freedom is $N_{DoF} = 2 - 0 - 2 = 0$.
- Sub-network 3 consist of **h2**, **c4**, **H**, **E2**, and **C**. The degrees of freedom is $N_{DoF} = 3 - 0 - 2 = 1$.
- Sub-network 4 consist of **c2** and **H**. The degrees of freedom is $N_{DoF} = 1 - 0 - 1 = 0$.

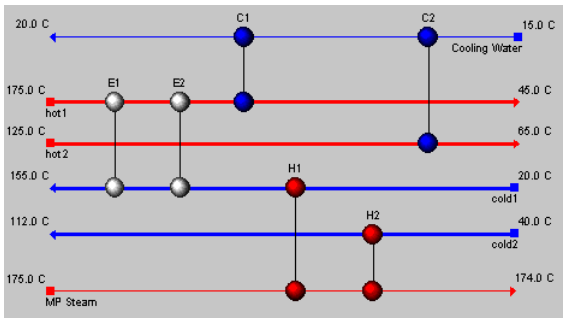
According to sub-network 1, the HEN design is actually lacking one manipulated variables for that particular sub-network.

Sub-networks and the utility system

Each utility stream can be included or not in a sub-network depending of its characteristics.

For example, consider the HEN design in the figure below:

Figure 6.48



- If both utility streams are included in the sub-networks identification, there is only one sub-network in the above HEN design. This sub-network contains the following streams: *hot1*, *hot2*, *cold1*, *cold2*, *MP Steam*, and *Cooling Water*.
- If the utility streams are not included, there are three sub-networks in the above HEN design. One of the sub-network contains the *cold2* stream, while another sub-network contains the *hot2* stream, and the final sub-network contains the *hot1* and *cold1* stream.

If a utility stream can be used to control the outlet temperature of more than one process stream, it should not be included in the sub-network. This option implies that disturbances are not propagated through the utility stream.

6.5 Data Extraction

One of the truly unique features of HX-Net is its ability to extract information from existing HYSYS cases or existing Aspen Plus backup files. This allows for an energy study to be performed on an existing plant which has been modeled in HYSYS or Aspen Plus.

The objective of the Data Extraction option is to allow you to compare the thermodynamically best possible use of energy with what you actually have in the plant.

6.5.1 Extraction Steps From HYSYS/Aspen Plus

The Data Extraction option uses seven steps to extract data from a HYSYS or Aspen Plus simulation.

Step 1 - Selecting Files

In the first step, you need to select the following three files:

By default, HX-Net provides its own *utility database* and *economic* files, however you can change these selected files.

- Utility Database file. The utilities data are not extracted from HYSYS or Aspen PLus, so you need to provide a separate utility database for HX-Net to assign utilities to the case from HYSYS or Aspen Plus.
- Economic file. You need to provide economic parameters for calculating the cost of heat exchangers.
- Simulation file. You need to provide the HYSYS file (*.hsc) or an Aspen Plus backup file (*.bkp) that contains the process information you want to extract from.

Step 2 - Set Options for Extraction

In the second step, you need to set the extraction options.

- You can select whether to segment the streams or not, and when to segment the streams.
- You can select to ignore or place heaters/coolers for pumps, recycles, and pipe segments that occur in the PFD.
- You can select whether to extract live steam or not and how much information about the live steam is extracted.

Live steam will be extracted as a process stream.

Refer to **Section 8.2.3 - Set Options Page** from the **Heat Integration** manual for more information about setting the extraction option.

Step 3 - Performing the Extraction

As a default setting, HX-Net selects all subflowsheets in the selected simulation.

In the third step, you can select the subflowsheets that contain the process information you want to extract from the HYSYS or Aspen Plus simulation.

In Aspen Plus, a separate subflowsheet is created for the main simulation and for each existing distillation column.

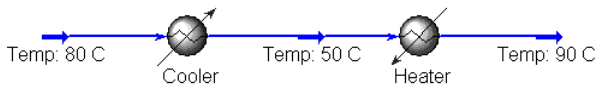
Then HX-Net performs the following multiple sub-steps as it begins extracting the process data from the HYSYS or Aspen Plus simulation.

1. First it is necessary to identify the streams that have the same composition. The difficulty is that the streams could have the same composition within a specified tolerance value.
2. The default relative tolerance value used is 0.001. However, in the case of HYSYS, if the recycle blocks have a greater tolerance value than the default value, then the value from the recycle block is used. HYSYS stores the tolerance as a multiplier (see the HYSYS reference manual)
3. Flowsheet streams are grouped by composition using the tolerance value determined above.
4. Each group of flowsheet streams with the same composition is scanned to identify those that belong to the same heat integration stream.

5. Next, splitter-mixer combinations and streams with temperature reversals are checked for:

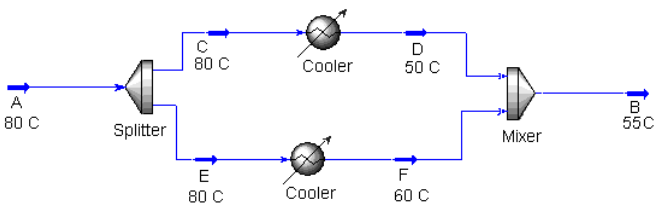
   - **Temperature Reversals**. This is where the temperature gradient of a stream changes direction at some point. For example, when a stream starts off with a high temperature and is cooled down and then heats back up (see figure below). HX-Net only deals with streams with a single temperature gradient. So, the groups of flowsheet streams are examined and if the temperature gradient changes direction, then that group of flowsheet streams is broken up into separate groups. In a way, two streams are created in HX-Net to handle the change of direction in the temperature gradient.

Figure 6.49



   - **Splitter Mixer Combinations.** Each group of flowsheet streams is examined to see if there is an acceptable splitter/mixer combination (see figure below). When two are found the corresponding flowsheet streams are used to fill in the branches.

Figure 6.50

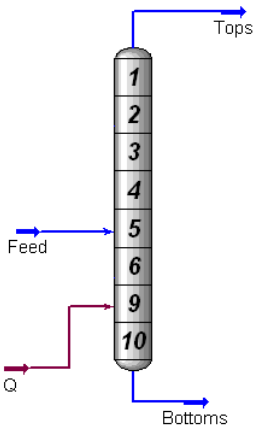


6. Process streams are then added to HX-Net. Process streams represent the groups of flowsheet streams that were created. The names used in HX-Net for these new streams consist of the inlet (first) and outlet (last) name of the flowsheet streams in that group separated by '_TO_'.
7. When process streams are extracted from HYSYS or Aspen Plus to HX-Net certain properties of the stream are extracted as well. These are: mass flowrate, total heat load, temperature, viscosity, density, thermal conductivity, and effective heat capacity.
8. A process stream has an associated temperature gradient. The temperature change could affect some of the stream properties. For example, everything will not always be constant throughout the

stream. HX-Net accounts for this by segmenting the stream into different temperature regions each with their own set of properties. HYSYS or Aspen Plus have multiple flowsheet streams for any given process stream; meaning that the properties at several temperatures are known. Using the variation that is seen in HYSYS or Aspen Plus, HX-Net decides where and when to segment a stream. HX-Net uses enthalpy values for segmenting. On account of this the heat capacity values in HX-Net can appear differently from the original values in HYSYS or Aspen Plus because the latent heat is accounted for.

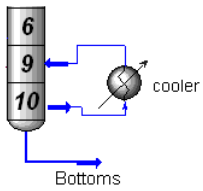
9. Next, special cases are checked: Live Steam, Reboilers and Condensers, and Energy Streams.

   - **Live Steam**. It is steam fed into a process. HX-Net treats this as a separate process stream. HX-Net accounts for the fact that this steam has to come from somewhere. To do this, a process stream is created that has an inlet temperature of 20^{o}C (ambient) and an outlet temperature of that of the flowsheet stream.
   - In order to make a fair comparison between targets and design live steam must be accounted for in the design as well. It is matched with a utility stream that is most suitable. The capital cost of this match is set to zero. This is because in a real network the live steam will not be matching the utility inside the plant but will be generated in the utility system.
   - **Reboilers and Condensers.** All reboilers and condensers are now accounted for.
   - **Energy Streams.** This accounts for tray draws and flashes with energy streams.
   - **Tray Draw**. HYSYS or Aspen Plus allows the addition of an energy stream to the middle of a column. It is perfectly acceptable, for example, to have a column that has an energy stream entering on the tenth stage. HX-Net does not deal with energy streams, only with process and utility streams. In the absence of more information an assumption is made as to what this energy stream physically represents:
     The assumption is that physically there is a draw from the column on either the eighth or tenth stage depending on the sign, negative or positive respectively, of the Q for the energy stream. A negative Q, the removal of heat, indicates that vapour is drawn from the tenth tray and is passed through a heat exchanger



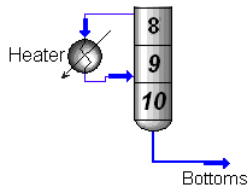
before being returned to the ninth tray at a lower temperature.

Figure 6.51



A positive Q, the addition of heat, indicates that liquid is removed from the eighth tray and passed through a heat exchanger before being returned to the ninth tray at a higher temperature.

Figure 6.52



No matter which of the two scenarios above is taking place, two streams will be used in HX-Net. A process stream will be created to represent the draw from the column and its return. The heating or cooling requirement of the process stream will be satisfied with a utility stream.

For heat integration purposes, it is best to simulate a column in HYSYS or Aspen Plus with real heat exchangers. For example, through pump arounds/pump backs to represent energy going into or out of a column, instead of using energy streams.

- **Flash With An Energy Stream.** In HYSYS or Aspen Plus, this occurs when a flash happens and an energy stream is involved. That is, where there is a flash with a net gain or loss of energy, which is dealt with via an energy stream. Essentially, this occurrence is dealt like a heat exchanger in HX-Net. This assumption is made due to the lack of further information about the actual physical representation.
- **Unit operation with multiple inlets**. In the case of Aspen Plus, unit operations may have multiple inlets which are internally mixed before the operation is performed. HX-Net represents this

situation by extracting a mixer that combines the multiple inlet streams into a single stream. The new single inlet stream's properties are obtained by flashing the mixture of inlet streams.

10. Next, the heat exchanger network is constructed. A list of all the heat exchangers, heaters, and coolers that were extracted from the HYSYS or Aspen Plus simulation is created. Then these lists are traversed and the heat exchangers, heaters and coolers are added to the network. To do this, HX-Net needs Utility streams:

    - In HYSYS or Aspen Plus, you can have an energy stream attached to a heat exchanger indicating whether or not energy is being added or removed. HX-Net does not deal with energy streams, so it replaces the energy streams with utility streams.
    - Utility streams are added based on the temperature on the process stream it is to be used with. There is a set of 20 default utilities that are used during extraction (see figure below). Each utility in the list has an Applicable Range High (ARH) and an Applicable Range Low (ARL) value. It is this "Applicability Range" that determines which utility is used.

Figure 6.53

Utility Database

Hold

Name	Inlet T [C]	Outlet T [C]	HTC [kJ/h-m2-C]	Cost Index [Cost/kcal]	ARH [C]	ARL [C]	DTmin [C]	Viscosity [cP]	Conductivity [W/m-K]	Density [kg/m3]	Eff. Cp [kJ/kg-C]	Type
LP Steam	125.0	124.0	2.160e+004	7.950e-006	115.5	-26.50	10.00	0.013	0.027	558.00	2196.40	Steam Reboiler
MP Steam	175.0	174.0	2.160e+004	9.205e-006	165.5	115.5	10.00	0.015	0.031	493.00	1981.40	Steam Reboiler
HP Steam	250.0	249.0	2.160e+004	1.046e-005	240.5	165.5	10.00	0.018	0.038	421.00	1703.10	Steam Reboiler
Hot Oil	280.0	250.0	836.2	1.464e-005	275.5	240.5	5.000	10.000	0.170	820.00	3.000	Shell & Tube
Fired Heat (1000)	1000	400.0	399.6	1.778e-005	975.5	275.5	25.00	0.000	0.000	1.23	1.000	Fired Heater
Fired Heat (2000)	2000	400.0	399.6	2.653e-005	1971	975.5	30.00	0.000	0.000	1.23	1.000	Fired Heater
Very High Temperature	3000	2999	399.6	3.724e-005	2991	1971	10.00	0.000	0.000	1.23	1.000	Fired Heater
Refrigerant 1 Generation	-24.00	-25.00	4680	-1.134e-005	-26.50	-41.50	3.000	5.500	0.560	1200.00	4.000	Shell & Tube
Refrigerant 2 Generation	-39.00	-40.00	4680	-1.393e-005	-41.50	-65.50	3.000	0.007	0.012	2.27	1.341	Shell & Tube
Refrigerant 3 Generation	-64.00	-65.00	4680	-2.433e-005	-65.50	-103.5	2.000	0.007	0.012	2.27	1.341	Shell & Tube
Refrigerant 4 Generation	-102.0	-103.0	4680	-3.534e-005	-103.5	-273.1	2.000	0.007	0.012	2.27	1.341	Shell & Tube
Cooling Water	20.00	25.00	1.350e+004	8.889e-007	44.50	29.50	5.000	1.000	0.603	998.00	4.183	Shell & Tube
Air	30.00	35.00	399.6	0.0000	134.5	44.50	10.00	0.000	0.000	1.23	1.000	Air Cooler
LP Steam Generation	124.0	125.0	2.160e+004	-7.908e-006	184.5	134.5	10.00	0.013	0.027	558.00	2196.40	Steam Generator
MP Steam Generation	174.0	175.0	2.160e+004	-9.163e-006	259.5	184.5	10.00	0.015	0.031	493.00	1981.40	Steam Generator
HP Steam Generation	249.0	250.0	2.160e+004	-1.042e-005	3000	259.5	10.00	0.018	0.038	421.00	1703.10	Steam Generator
Refrigerant 1	-25.00	-24.00	4680	1.146e-005	29.50	-21.50	3.000	5.500	0.560	1200.00	4.000	Shell & Tube
Refrigerant 2	-40.00	-39.00	4680	1.408e-005	-21.50	-36.50	3.000	0.007	0.012	2.27	1.341	Shell & Tube
Refrigerant 3	-65.00	-64.00	4680	2.458e-005	-36.50	-62.50	2.000	0.007	0.012	2.27	1.341	Shell & Tube
Refrigerant 4	-103.0	-102.0	4680	3.569e-005	-62.50	-100.5	2.000	0.007	0.012	2.27	1.341	Shell & Tube
Very Low Temperature	-270.0	-269.0	4680	3.724e-005	-100.5	-267.5	2.000	0.007	0.012	2.27	1.341	Shell & Tube
New	---	---	---	---	---	---	---	---	---	---	---	Shell & Tube

    - If the process stream enters at 80^{o}C and leaves at 35^{o}C, then the utility stream that would be chosen by HX-Net would be Cooling Water. This is because the Applicable Range for Cooling Water is 135^{o}C to 30^{o}C and the process stream clearly falls within this range.

11. HX-Net provides a default economic data set, which is invoked when data is extracted from HYSYS or Aspen Plus if no other set has been provided.

12. Range Targeting is now performed and an optimal range for the DTmin is determined. The average of this optimal range is calculated. Targets are then calculated using the average as the DTmin value.

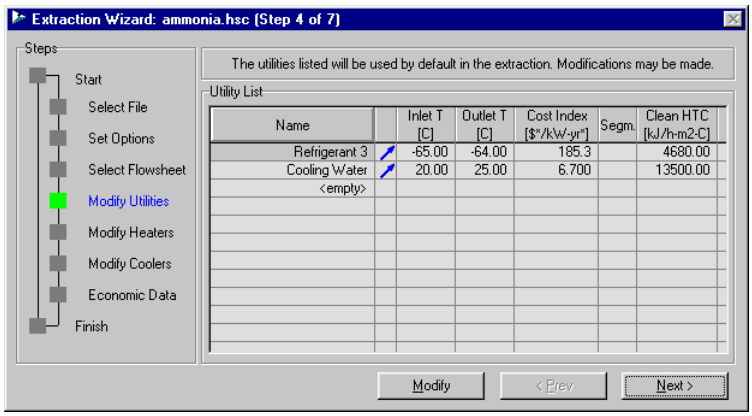
Step 4 - Selecting Possible Utilities

In the fourth step, HX-Net presents a list of possible default utilities to be used for cooling and/or heating the process streams.

You can add and modify the list of utilities available for the HEN to better reflect the utilities used in the plant process.

For example, Data Extraction option selected Refrigerant 3 and Cooling Water for the cooling utilities.

Figure 6.54



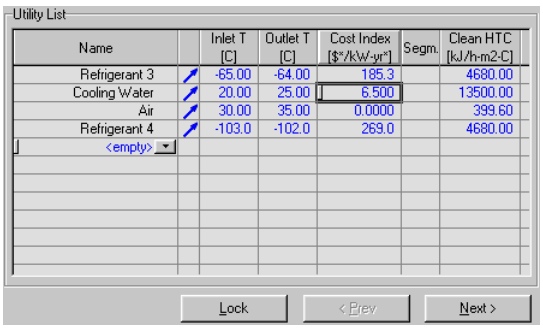
Your plant, however, may have cooling water, air, and Refrigerant 4. The cost value of cooling water may also be different.

The text in the Utility List table turn blue in colour, indicating you can modify the information in those text.

1. Click the **Modify** button.
2. Enter the cost value of the cooling water for your plant in the appropriate cell under the Cost Index column.
3. Click the down arrow in the **<empty>** cell to open the drop-down list and select **Air** from the list.

4. Repeat the above procedure for **Refrigerant 4**.

Figure 6.55



5. Click the **Lock** button to set/fixed the new list of utilities for the HEN.

Step 5 - Modify the Hot Utilities Connection

In the fifth step, you can modify/change the hot utilities connected to the heaters in the HEN. The ability to modify the hot utilities allows the hot utilities connection in the HEN more accurately reflect the hot utilities connection in the plant.

Step 6 - Modify the Cold Utilities Connection

In the sixth step, you can modify/change the cold utilities connected to the coolers in the HEN. The ability to modify the cold utilities allows the cold utilities connection in the HEN more accurately reflect the cold utilities connection in the plant.

Step 7 - Selecting the Economic Cost Set

In the seventh step, you can modify and associate certain economic set to certain heat exchangers in the HEN. This ability provides reasonable estimate of the capital cost of the HEN.

6.5.2 Summary Report

After the data extraction has been completed, HX-Net will generate a report on the data extraction and display it on the *Report* tab of the Summary view.

HX-Net will also calculate and display some key variable values for both optimum/target performance and the current HEN design in the *Summary* tab of the Summary view. So you can compare the optimum design with the current design of the plant.

Warnings and Limitations

The *Report* tab of the Summary view contains a warning section. In this section of the report, a list of all possible problems will be displayed.

The following paragraphs deals with all of the warnings that can occur, along with a few limitations in data extraction that do not have a warning.

Tolerances

“Composition tolerance too high. Recommended value is 1 or lower. Extraction results may be erroneous”

In many HYSYS flowsheets, a Recycle block can exist. By default, the tolerances for solving the Recycle are set to 10, which may result in problems with the data extraction to HX-Net. To solve this problem, return to HYSYS and modify the Recycle block so that the tolerances are below 1. Make sure that the flowsheet still solves, or the data will not be extracted properly either. Once the flowsheet is solving at the lower tolerances, perform the data extraction again.

Temperature Reversal

"Stream is being first heated and then cooled, or vice-versa"

An example of this occurring in HYSYS or Aspen Plus would be a material stream that first passes through a cooler, goes through a couple of other operations, and then passes through a heater. HX-Net will split this stream into two. Not much can be done in this case to remedy the problem in HYSYS or Aspen Plus. The purpose of this warning note is to bring awareness to how HX-Net handles the problem.

Multiple Attachments

"Stream **streamName** in your simulation has multiple attachments. It is attached to: **UnitOperations....**"

In HYSYS, it is possible to have a stream with multiple attachments. For example, if you want to simulate the possibility of having either one large heater, or two smaller heaters in series, you can allow the inlet stream to have multiple attachments. HX-Net may extract this stream twice, resulting in inaccurate target calculations.

Multiple Feeds

*"**UnitOperationName** is a **UnitOperationType** with # feeds. Extraction results may be erroneous. Use a mixer to mix all the feeds before the reboiler."*

In the column subflowsheet environment, the reboiler and condenser unit operations allow multiple feeds. HX-Net will not correctly extract all of the inlet streams. To fix this problem, return to HYSYS, disconnect all of the inlet streams, send them to a mixer, and connect the mixer outlet stream to the condenser or reboiler. Double check that the entire flowsheet still solves before re-extracting the data into HX-Net.

LNG Exchangers

“LNG exchangers were found in your simulation. These have not been considered in the heat exchanger network. Please deal with them manually.”

HYSYS contains an LNG exchanger unit operation, which allows for heat transfer between multiple hot and multiple cold stream. HX-Net will extract the information for all stream entering and exiting the LNG Exchanger, but it will not place any heat exchangers on the Grid Diagram. To fix this problem you must return to HYSYS, and split each hot stream into the same number of branches as there are cold streams. For example, if there are 4 cold streams, split each hot stream into four streams by using a Tee unit operation. Then place a heat exchanger between every branch on each hot stream and each cold stream. If you were to have 5 hot streams with the 4 cold streams, you will end up with 20 heat exchangers being placed. As always, make sure that the HYSYS flowsheet solves completely before performing the data extraction in HX-Net.

Enthalpy Change Opposite to Temperature Change

“The direction of temperature change is not the same as the direction of enthalpy change. Typically, this is due to pressure changes in streams”.

If you have a high pressure gas stream that enters a heat exchanger, and it loses a great deal of pressure as it is cooled, you can have an increase in enthalpy while you have a decrease in temperature. This will tend to happen more with streams of almost pure components. HX-Net ignores streams such as these. To remedy the problem, return to HYSYS or Aspen Plus and replace the high pressure drop heat exchanger with a heat exchanger with no pressure drop, and a valve, to simulate the pressure drop. Solve the flowsheet before attempting the data extraction again.

Streams and Unit Operations with Same Names

In the case of HYSYS, although no warning message appears, HX-Net does not distinguish between streams and unit operations with the same names. If your network after simulation is not satisfied, or missing a stream or heat exchanger, check your HYSYS simulation to make sure that there are no duplicated names.

In the case of Aspen Plus, the process streams are extracted after all the unit operations have been extracted. Therefore, if a process stream has the same name as a previously extracted unit operation, HX-Net adds the identifier (**stream**) to the process stream's name.

6.5.3 Extraction Tips

The following tips should be read to ensure that an accurate automated data extraction is performed.

1. Do you have unnecessary streams or unit operations in the simulation case?
   - **Comment:** HX-Net will extract the data of all unit operations and streams present in the simulation case. These unnecessary unit operations and streams can lead to the wrong target calculations by HX-Net.
   - **Tip:** Remove the unnecessary unit operations and streams from the simulation case or update the process stream data appropriately.
2. Are all the unit operations and streams converged in the simulation case?
   - **Comment:** If the unit operations and streams are not converged (in the case of Aspen Plus, the calculations are completed with errors), HX-Net will extract the streams as incomplete (i.e. no inlet temperature and/or no outlet temperature and/or no streams at all) and will not be able to place any heat exchangers on these streams. You will have to place the heat exchangers manually.
   - **Tip:** Make sure that all unit operations and streams are converged in the simulation case.
3. Are you using HYSYS in dynamic mode?
   - **Comment:** When HYSYS is running in dynamic mode, the properties of streams and unit operations are changing over time. HX-Net ignores streams and unit operations with changing properties. A warning will appear in the summary report.
   - **Tip:** Set HYSYS to run in steady state mode.

4. Do you have streams with enthalpy increase (decrease) but temperature decrease (increase) due to pressure drop in your simulation case? For example, a high-pressure gas stream is heated in a heat exchanger with a considerable pressure drop.
   - **Comment:** These streams are ignored by HX-Net. A warning will appear in the summary report.
   - **Tip:** Model these systems with a heat exchanger with no pressure drop and a valve (pump/compressor) to achieve the desired behaviour.
5. Are there any internal streams present in your HYSYS simulation case (internal streams are duplicates which can be created in the column environment)?
   - **Comment:** HX-Net makes no distinction between internal and real streams. It will extract internal streams as real streams. If there is a heat exchanger placed on the internal stream, it will also be extracted.
   - **Tip:** Avoid the use of internal streams in HYSYS. If the simulation must have internal streams, then extract the data and delete the undesired duplicates.
6. Do you have recycles in your HYSYS simulation case with loose tolerances on temperatures, etc.?
   - **Comment:** HX-Net breaks the stream at a Recycle unit with big temperature differences between inlet and outlet temperatures.
   - **Tip:** Reduce the tolerances of the Recycle in HYSYS or merge the streams manually in HX-Net.
7. Do you have any utilities modelled as part of the simulation case?
   - **Comment:** HX-Net assumes that all the streams present in the HYSYS or Aspen Plus simulation are process streams.
   - **Tip:** Remove any utility streams from the simulation case and specify them as utility streams in HX-Net or edit the data in HX-Net.
8. Do you have process streams spanning across multiple flowsheets in your HYSYS simulation?
   - **Comment:** HX-Net considers the portions of streams in different flowsheets as different streams.
   - **Tip:** Ensure that all the heat exchangers are part of the same sub-flowsheet. If this cannot be done, then merge the streams in HX-Net.

9. Do you have unit operations or streams that have the same name within the flowsheet or the sub-flowsheet in your HYSYS simulation?
    - **Comment:** HX-Net will not extract data from the streams and unit operations sharing the same name, for example a heat exchanger E1 with an energy stream of the same name.
    - **Tip:** Ensure that the names are not duplicated for every flowsheet/sub-flowsheet. This can be easily checked: click on select objects in the HYSYS's **PFD** menu for all the flowsheet and sub-flowsheets. The streams and unit operations are then displayed alphabetically ordered. Duplicate names will appear consecutive to each other in the list.
10. Do you have stand-alone non-isothermal mixers in your simulation case?
    - **Comment:** A stand-alone mixer in your simulation is a mixer that does not originate from a splitter (tee). HX-Net will ignore stand-alone non-isothermal mixing for heat integration. Notice the splitter/mixer combination, where a stream is first split, then performs the heat exchange and later mixes back again is extracted.
    - **Tip:** Model the stand-alone non-isothermal mixer as a combination of isothermal mixer and adjusting the temperature of the streams before/after the mixer with an appropriate heater or cooler.
11. Is your simulation a very large and complicated case?
    - **Comment:** There is no limitation on the size of the case that HX-Net can handle. However, HX-Net assumes that the case is solved when it starts the data extraction. If HYSYS needs a few iterations to solve the case, or in the case of Aspen Plus, the case has not been run to completion, HX-Net might start the extraction process too early resulting in an incorrect extraction.
    - **Tip:** Open the case in HYSYS first and allow it to solve, or open the Aspen Plus backup file and run it to completion. Once the case has converged or run to completion, select the simulation file and extract normally.
12. Do you have LNG exchangers in your simulation?
    - **Comment:** HX-Net will extract the streams but not the LNG exchanger as multistreams heat exchangers are not supported by HX-Net. This will have no effect on the energy targets of the process.
    - **Tip:** The LNG exchangers are not considered in the heat exchanger network and must be dealt with manually. For an LNG exchanger between m hot and n cold streams, split each hot stream into n branches. Place an exchanger between each branch on that stream with every cold stream, and vice versa.

13. Streams will be extracted incorrectly if they span through sub-flowsheets and are connected to different unit operations with the same name in your HYSYS case.
    For example, consider Stream1 starts in Sub-Flowsheet A and ends in Sub-Flowsheet B. Inside Sub-Flowsheet A, Stream1 is connected to a heat exchanger E-100. There will be a problem if Sub-Flowsheet B also contains a heat exchanger named E-100 and Stream1 is connected to it.
    - **Tip:** Rename one of the unit operations that share the same name in your HYSYS case.
14. Do you have short cut columns in your simulation?
    - **Comment:** A short cut column will cause the physical properties in the related streams to be very approximate.
    - **Tip:** For a better physical property approximation use real columns in your simulation.
15. Do you have streams with multiple attachments?
    - **Comment:** HYSYS steady state allows the user to attach a stream to several unit operations. Only one attachment will get extracted properly into HX-Net. The extracted heat exchanger network will therefore be error-prone.
    - **Tip:** Do not attach a stream to several unit operations.

HX-Net uses a default set of utility and economic data to produce the summary view. The default set data may not be a true representation of the conditions of your project. You must edit the data to suit your economic conditions.

We recommend that you inspect the Report tab where the data extraction log is shown. The warning section will detail any difficulty encountered by HX-Net during the extraction process.

6.6 Parametric Optimization

The HEN optimization feature can be used in:

- the **design** mode for minimization of the heat transfer area or total annual cost.
- the **retrofit** mode for minimization of the payback period after a topology change in the network.

HX-Net employs a proprietary algorithm for non-linear optimization of heat exchanger networks (HENs). You must ensure that the model of the HEN is correctly and completely defined before running the optimization feature.

6.6.1 Optimization Algorithm

The optimization algorithm identifies the existing sub-networks and performs the optimization for each sub-network independently. For each sub-network, the algorithm selects the heat exchanger loads and split fractions that will be optimized in order to minimize the objective function.

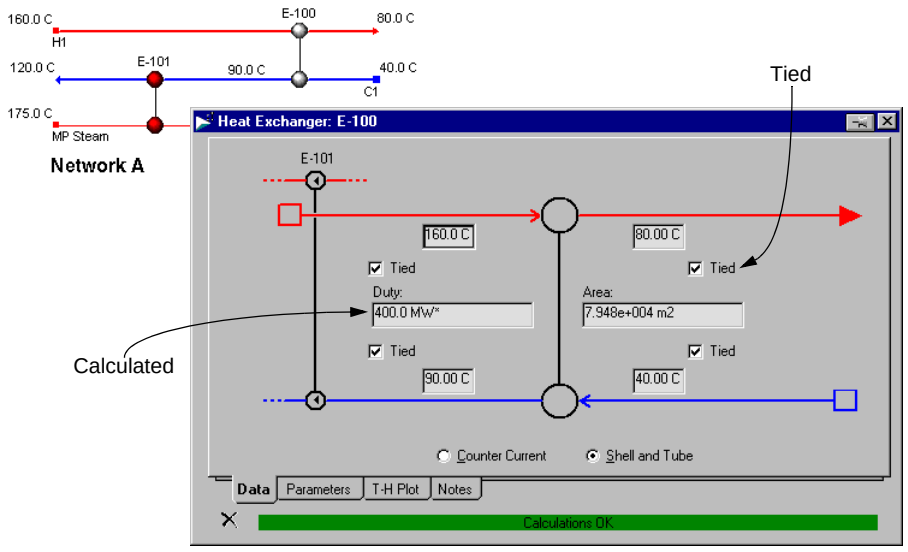
In the *design* mode, you have the choice of optimizing both load and split fraction or just one of them. In the *retrofit* mode, both variables are optimized simultaneously. All other specifications like *intermediate temperatures* and *outlet stream ties* will not be changed during the optimization. The algorithm tests and rejects infeasible designs as final solutions.

6.6.2 Specifying the Network Task

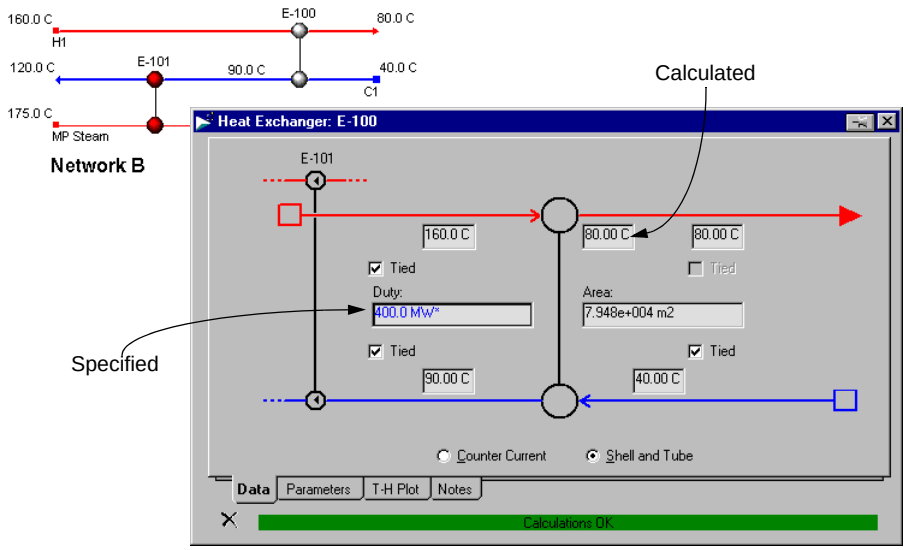
A HEN is designed to accomplish a specific task, to promote a certain amount of heat/duty exchange so that all process streams attain their specified outlet temperatures. The initial model of the HEN must take into account this task. The best way to specify a HEN is tying all outlet temperatures. If the outlet temperature of a process stream is not tied, the optimizer will not treat this outlet temperature as a specification. As a result, the exiting stream from the optimized heat exchanger may have a different temperature from the specified outlet temperature.

The following example presents the same HEN specified in two different ways.

Figure 6.56



In the HEN A, the load of heat exchanger E-100 was calculated based on the temperature values of the inlet and outlet streams.



In the HEN B, the load of the heat exchanger E-100 was specified and the outlet temperature of the stream H1 was calculated.

For the HEN A, the optimizer will not attempt to change the load of E-100, because this value was calculated from the specified temperatures. For the HEN B, however, the outlet temperature of stream H1 was not specified (tied), so the optimizer will attempt to optimize the load of E-100. Consequently, the outlet temperature of stream H1 will be changed during the optimization.

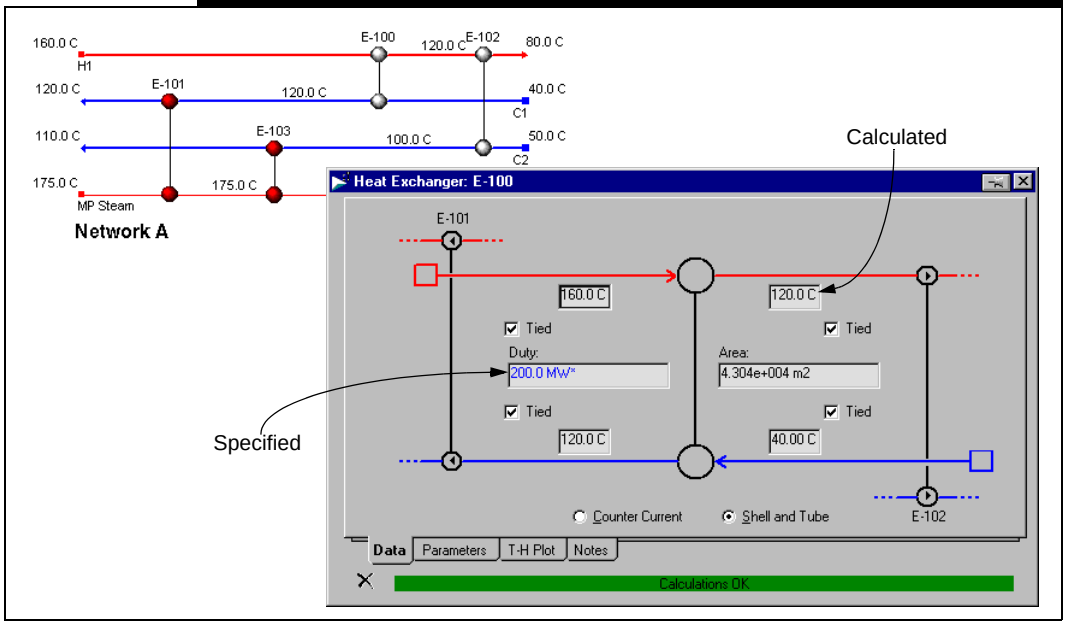
Tying all outlet temperatures guarantees that all process streams are satisfied in the final solution.

6.6.3 Temperature Specifications in the Network

All specified intermediate temperatures in the HEN will be treated as hard constraints and they will not be changed during the optimization. Caution must be taken when an internal temperature is specified because the specified temperature reduce the scope for optimization.

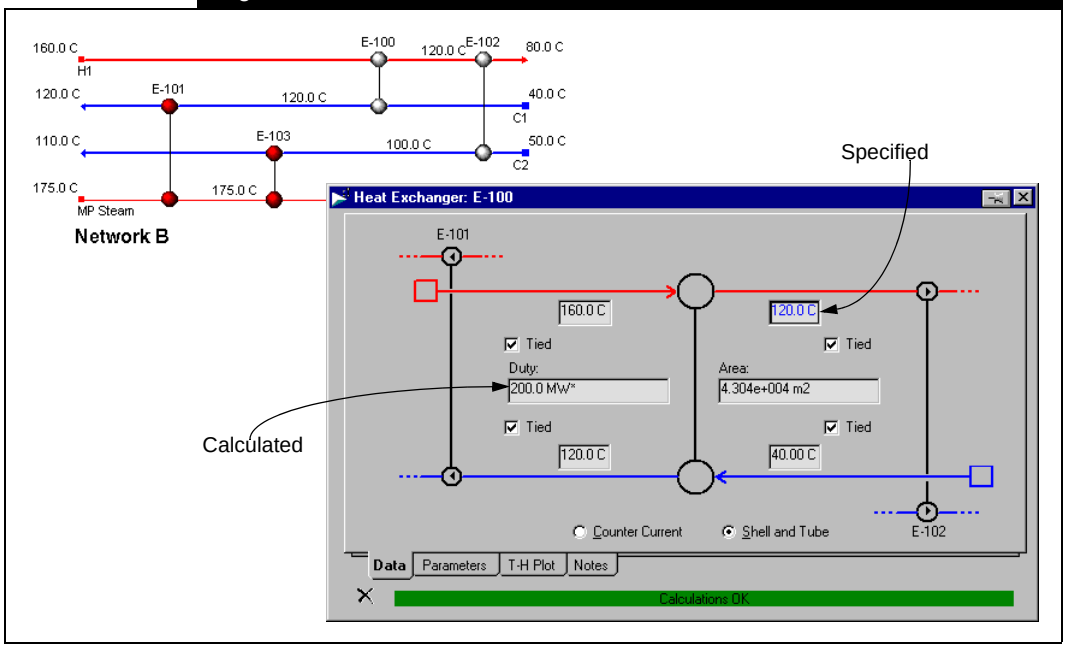
The following example shows why specified internal temperatures should be avoided.

Figure 6.57



In HEN A, all outlet temperatures are tied. From a degree of freedom analysis, it is possible to conclude that one duty must be specified. If for instance, the duty of heat exchanger E-100 is specified as 200.0 MW, the duty of heat exchanger E-102 is calculated to satisfy the total load of stream H1. The duty of E-100 can be optimized in order to minimize a given objective function.

Figure 6.58



In HEN B, the temperature of the node between heat exchangers E-100 and E-102 is specified as 120°C, and all duties are calculated. During optimization, the temperature specified will be kept and therefore no load can changed/modified for optimization. It can be concluded that specifying intermediate temperature decreases the scope of optimization. The possibility of keeping the specified intermediate temperatures is a flexible feature of the optimization algorithm, however, you must be aware of its implications.

6.6.4 Optimization Wizard

The Optimization Wizard is an assistant that helps you to check if the HEN is correctly defined. The following table lists all the critical items that are checked by the Optimization Wizard:

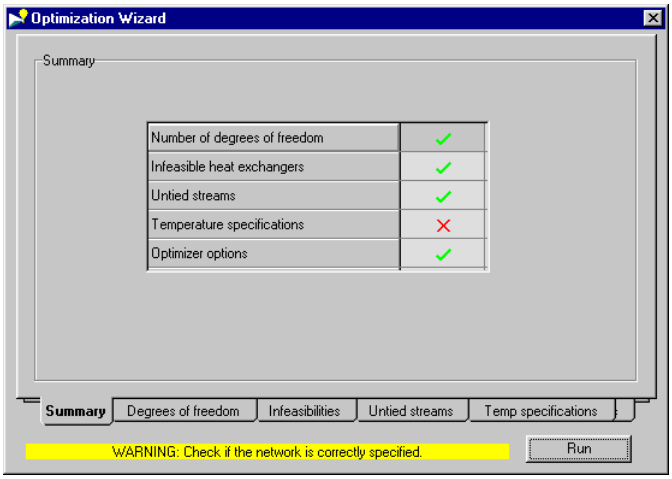
Item	Description	Implication
Degrees of Freedom	The overall number of degrees of freedom must equal 0 (i.e., the overall network must be correctly specified). All heat exchangers calculation status must be complete. The Optimization Wizard will check if there are any heat exchangers that are partially calculated or overspecified.	The Optimizer feature cannot run if the degrees of freedom are not satisfied.
Infeasible Heat Exchangers	All heat exchangers in the HEN must be feasible	The Optimizer feature cannot run if there are infeasible heat exchangers.
Untied Intermediate Stream Temperatures	All intermediate stream temperatures between heat exchangers and/or splitters-mixers must be tied. No intermediate energy gap is allowed in the HEN.	The Optimizer feature cannot run if there are untied intermediate node temperatures.
Intermediate Stream Specifications	All temperature specification in the HEN are treated as hard constraints by the optimizer. The specified temperature reduces the scope for optimization, since there are less free heat exchanger loads to be used as optimization variables.	The Optimizer feature will run, however, a warning message will appear.
Untied Heat Exchanger Outlet Temperatures	Outlet temperatures from heat exchangers should be tied, so that all process streams' temperatures are satisfied. If the outlet temperature is not tied, the outlet temperature of a process stream may not be equal to the process stream's target value	The Optimizer feature will run, however, a warning message will appear.

The Optimization Wizard is split into six tabs. Each tab displays information that indicate whether or not the items/areas in the network need to be corrected in order for the Optimizer feature to run smoothly.

Summary Tab

The Summary tab displays the status of the critical items checked by the Optimizer feature before attempting to perform optimization on the HEN design.

Figure 6.59

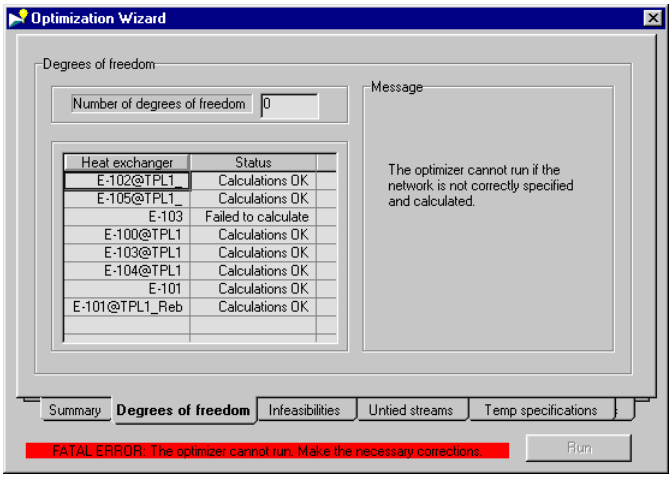


Green checkmark indicates that the status of the critical item is okay. Red X indicates that there are some unresolved issues in the critical item.

Degrees of Freedom Tab

The Degrees of Freedom tab displays the overall degree of freedom value and the calculation status of all the heat exchangers in the HEN design.

Figure 6.60

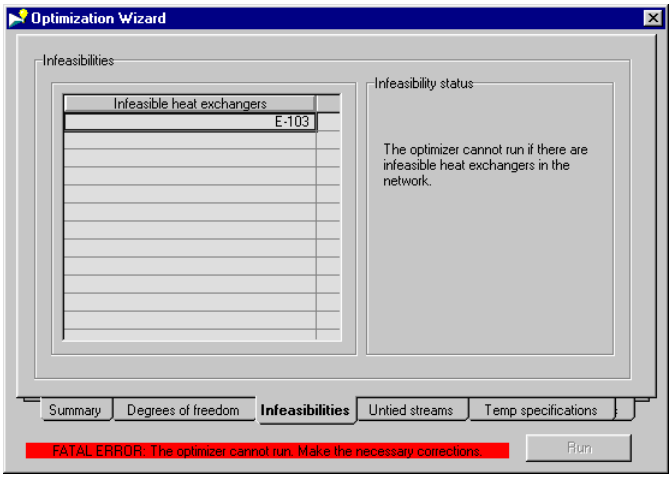


The Message group displays the status of the HEN design in terms of degrees of freedom.

Infeasibilities Tab

The Infeasibilities tab displays the name of any infeasible heat exchanger in the HEN design.

Figure 6.61

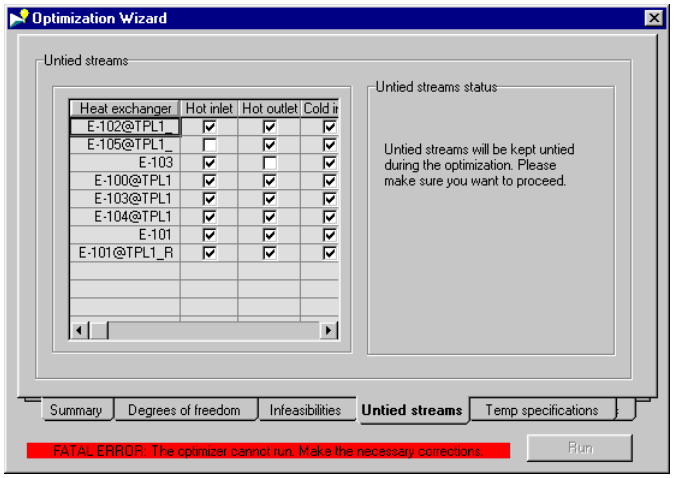


The Infeasibility status group displays the status of the HEN design in terms of feasible/infeasible heat exchangers.

Untied Streams Tab

The Untied Streams tab displays whether the inlet and outlet streams of the heat exchangers in the HEN design are tied or not.

Figure 6.62



The Untied streams group contains a table that displays the following information:

Checked checkbox indicates that the temperature of the stream is tied.

Unchecked checkbox indicates that the temperature of the stream is not tied.

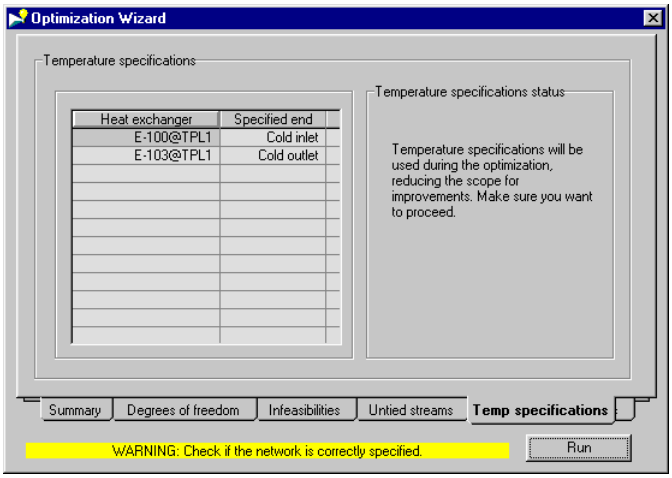
- The **Heat exchanger** column contains the names of all the heat exchangers in the HEN design.
- The **Hot Inlet** column indicates whether the temperature of the hot stream entering the exchanger is tied or not.
- The **Hot Outlet** column indicates whether the temperature of the hot stream exiting the exchanger is tied or not.
- The **Cold Inlet** column indicates whether the temperature of the cold stream entering the exchanger is tied or not.
- The **Cold Outlet** column indicates whether the temperature of the cold stream exiting the exchanger is tied or not.

The Untied stream status group displays the status of the HEN in terms of tied/untied streams.

Temp Specifications Tab

The Temp Specifications tab displays any heat exchanger that have specified temperature values.

Figure 6.63



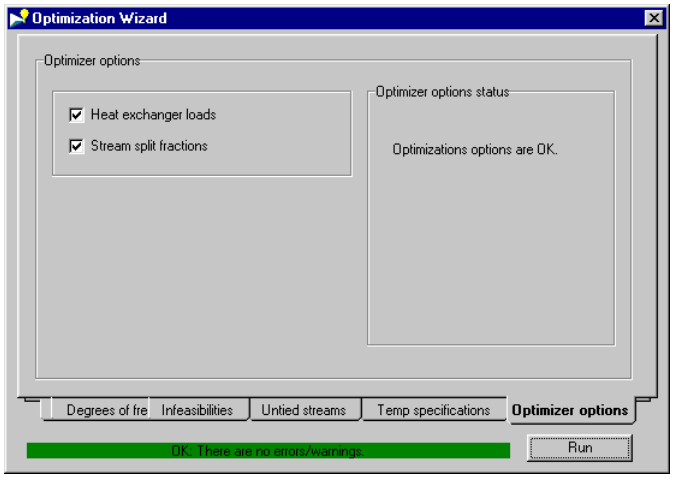
The heat exchanger name and specified temperature value is displayed in the *Heat Exchanger* and *Specified End* columns respectively.

The Temperature specifications status group displays the status of the HEN in terms of specified temperatures.

Optimizer Options Tab

The Optimizer Options tab allows you to modify how the HEN will be optimized.

Figure 6.64



Checked checkbox indicates the variable can be modified. Unchecked checkbox indicates the variable cannot be modified.

In the Optimizer options group, select the variables that are allowed to be modified during the optimization calculation. The two variables are heat exchanger loads and stream split fractions.

The Optimizer options status group displays the status of the optimizer option selection.

6.6.5 Optimizing a Network

To optimize the heat exchanger network (HEN):

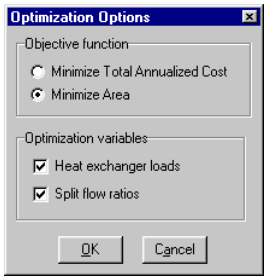
1. Open the HI Case or HI Project view.
2. Access the Grid Diagram of the operation:
   - For HI Case operation, click the **Open HEN Grid Diagram** icon to open the HEN Design view. Select the **Grid Diagram** tab to access the Grid Diagram.
   - For HI Project operation, select the Design you want to optimize from the Viewer group. The Grid Diagram will appear in the Main pane.
3. Click the **Open Palette View** icon to access the Grid Diagram Palette.
4. Click the **Open Optimization View** icon to access the Optimization Options view.

Open HEN Grid DIagram icon

Open Palette View icon

Open Optimization View icon

Figure 6.65



5. Choose which objective function you want to minimize by selecting the appropriate radio button in the Objective Function group.
6. Select the optimization variables you want the Optimizer feature to change when preforming the optimization.
7. Click the **OK** button.
8. The Optimization Wizard view will appear.
   Refer to **Section 6.6.4 - Optimization Wizard** for more information.
9. Check all the items that may affect the Optimizer feature's calculation, and make any necessary changes to the HEN.
10. Click the **Run** button. The selected HEN design will be optimized.

Check the checkbox to allow modification on the associate variable. Uncheck the checkbox to forbid modification on the associate variable.

6.6.6 Optimization Results

If you perform optimization in a HI Case operation, the starting design is replaced by the optimized design. In HI Project a new design with "-O" attached to the design name. The attached "-O" is to remind the user that the design was created by the Optimization Wizard feature.

6.6.7 Optimization Tips and Tricks

The following is a list of tips and questions when optimizing the heat exchanger network (HEN).

1. Check you specifications before you try to optimize the HEN.

   Optimizer feature treats load and area specifications in the same manner (i.e., the existing value will be overridden by the *optimized* value). In retrofit mode, it is possible to select which heat exchangers have their areas locked, thus Optimizer cannot change those locked areas.

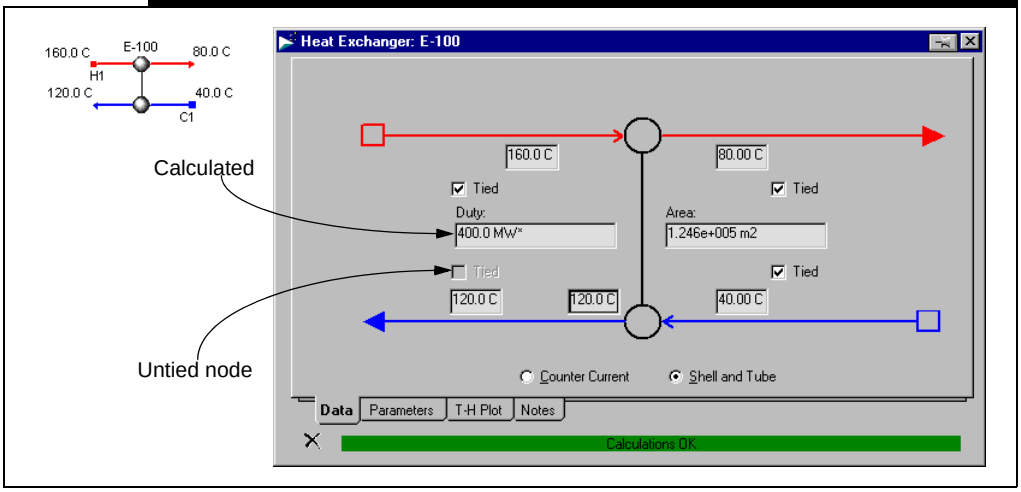
2. Simplify the HEN.

   Making the HEN simpler helps the Optimizer achieve the final solution faster. If you are not in the retrofit mode, removing the process streams which only exchange heat with utilities will also help the Optimizer obtain the final solution faster. For a quick screening of alternatives, try to specify the heat exchangers as counter-current type instead of 1-2 type.

3. What happens if it is not possible to tie all the outlet temperature?

   In some cases, as shown in the figure below, it is not possible to tie all end stream nodes temperature, due to the number of degrees of freedom.

Figure 6.66



In the above figure, the heat exchanger duty is calculated from the required load of stream H1, and the outlet temperature of stream C1 is also calculated. The load of this heat exchanger is not *free* to be changed, so the Optimizer will not attempt to optimize the load. So during the optimization, the outlet temperature of C1 will not change.

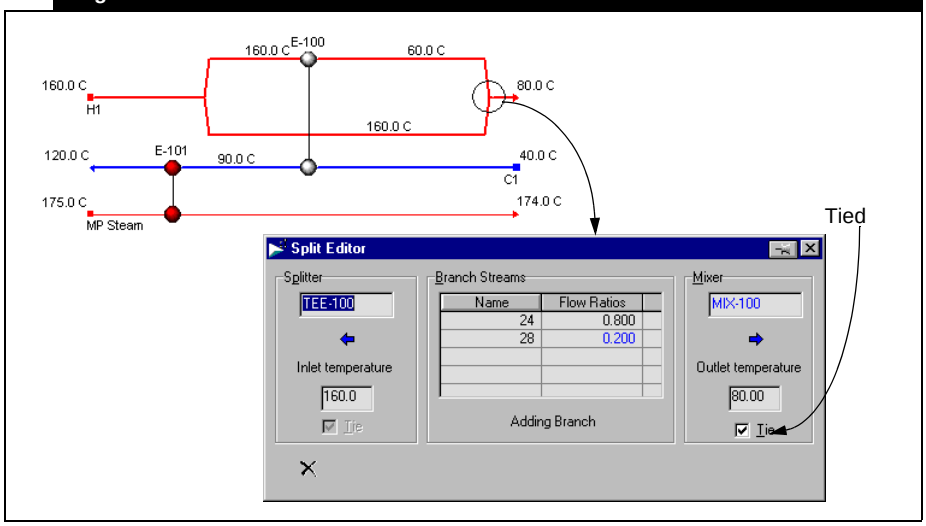
All heat exchanger loads that are calculated from temperature specifications or tied end nodes will not be optimized.

4. Is it possible to tie the outlet temperature of a mixer?

   Yes it is possible to tie the outlet temperature of a mixer. This option is particularly useful when a mixer is located in the end of a process stream.

From the figure below, the HEN contains a heat exchanger with a by-pass. As long as the outlet node of the mixer is tied, the outlet temperature of the process stream will not change in the final solution.

Figure 6.67

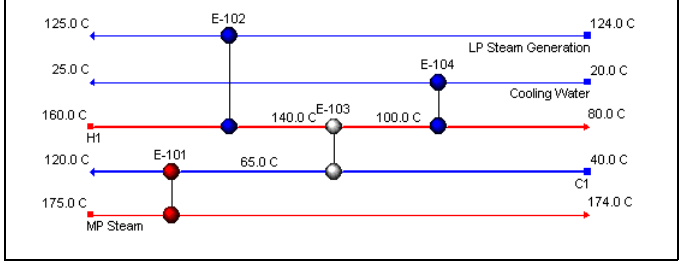


5. Does HX-Net optimize the best usage of different utilities attached to one process stream?

If for some reason it is not desired to change the balance between the two cold utilities, the temperature of the nodes around the utility heat exchangers must be specified.

Yes HX-Net does optimize the best usage of different utilities. It is very common to have more than one type of utility stream attached to a process stream, as shown in the figure below.

Figure 6.68



The H1 stream is cooled down using LP Steam Generation and Cold Water cold utilities. The Optimizer can be used to find the optimum balance between the two cold utilities.

7 Heat Integration - Operations Mode

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7.1 Introduction

The Operations Mode is a tool available in HX-Net for the analysis of the performance of an existing heat exchanger network (HEN) design when the operating conditions change. Decrease in the exchanger's heat transfer due to fouling, removal of an exchanger from service, changes in inlet temperatures or mass flowrate of process streams are among the possible operating variables you may consider to modify. Results showing the impact in the design are automatically provided when new values for one or more of these operating variables are entered.

Consider the process in **Figure 7.1** and the corresponding Grid Diagram in **Figure 7.2**.

Figure 7.1

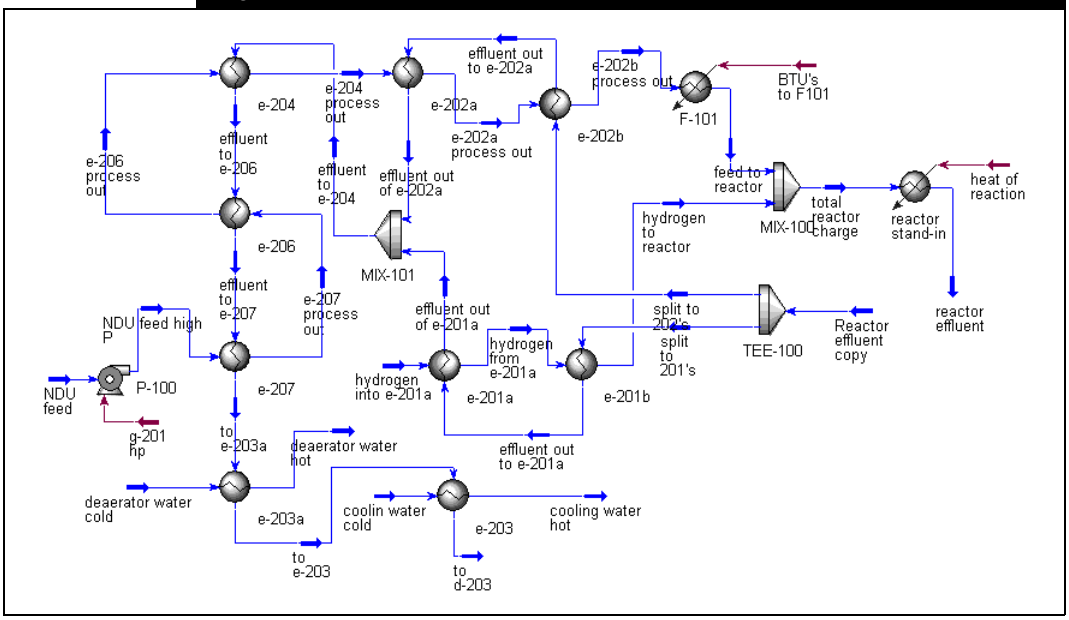
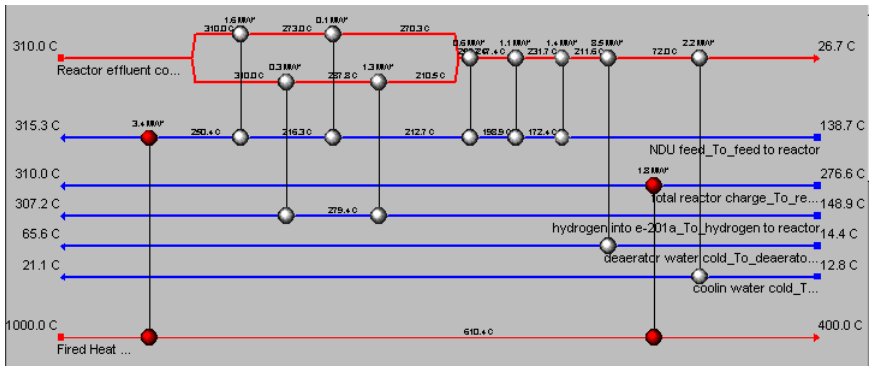


Figure 7.2



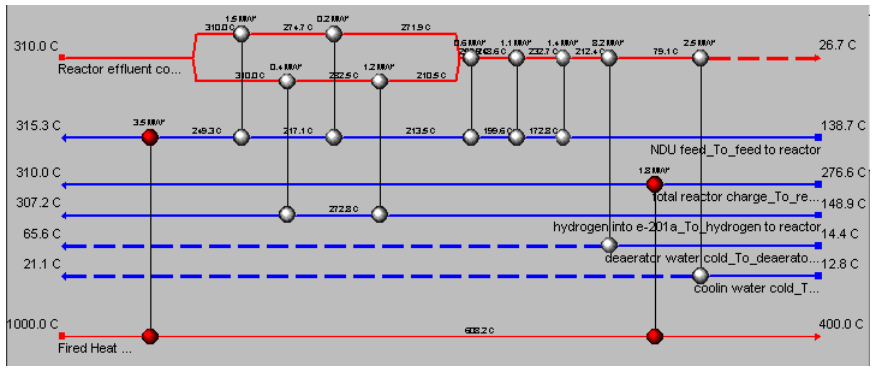
Refer to **Section 6.5 - Data Extraction** for more information about extraction.

This Grid Diagram has been obtained after extraction into a Heat Integration case from an existing HYSYS case. A sequential solver that calculates each heat exchanger individually and follows an iterative procedure is employed to solve the entire network.

Refer to **Section 3.1.1 - Entering Operations Mode** from the **Heat Integration** manual for more information about entering Operations mode.

Once the steps to enter Operations mode have been followed, the Operations Mode Grid Diagram is obtained. Notice that some of the streams become unsatisfied (dotted lines) since they are no longer able to reach their target temperatures.

Figure 7.3



In Operations Mode a simultaneous solver is employed that solves the entire system of equations at once and iterates to temperature convergence by updating the stream and heat exchanger physical properties (Rodera & Shethna, 2002[126]).

7.2 Basic Terminology

In order to properly analyse/simulate a heat exchanger network (HEN), a number of variables must be known. The variables are information about all streams containing energy, such as process and utility streams, and the economic parameter that will govern the cost calculations.

This section will describe briefly the basic terminology of the variables used to make up a HEN.

7.2.1 Process Streams

Refer to **Section 6.2.1 - Process Streams** for more information.

The process streams are the streams containing the fluid you want to heat or cool.

In Operations mode, the inlet temperature and mass flow rate values of the process streams are taken from the specified values in the Design mode. There are two types of outlet temperature for the process stream: Calculated and Target.

- The Calculated outlet temperature is a calculated value based on the specified conditions of the heat exchanger and inlet stream temperature.
- The Target outlet temperature is the specified/desired value from the Design mode.

For example, in a refinery plant the refinery operators try to maintain the crude outlet temperature from a heat exchanger at 330°C. Unfortunately, the crude outlet temperature from the exchanger is usually around 310°C due to fouling in the exchanger.

7.2.2 Utility Streams

Refer to **Section 6.2.2 - Utility Streams** for more information.

Utility streams are used to satisfy unsatisfied heating and/or cooling requirements of the process streams.

In Operations mode, the inlet and outlet temperature values of the utility stream is taken from the specified values in the Design mode. The required mass flow of the utility stream is calculated based on the total heat load of the utility (the sum of the loads of heaters/coolers attached to the utility stream).

The heat load and operating cost of the utility stream is also calculated.

7.2.3 Economic Parameters

Refer to **Section 6.2.6 - Economic Parameters** for more information.

The economic parameters are required to calculate the capital cost and the annualization factor of the heat exchangers in the heat exchanger network (HEN).

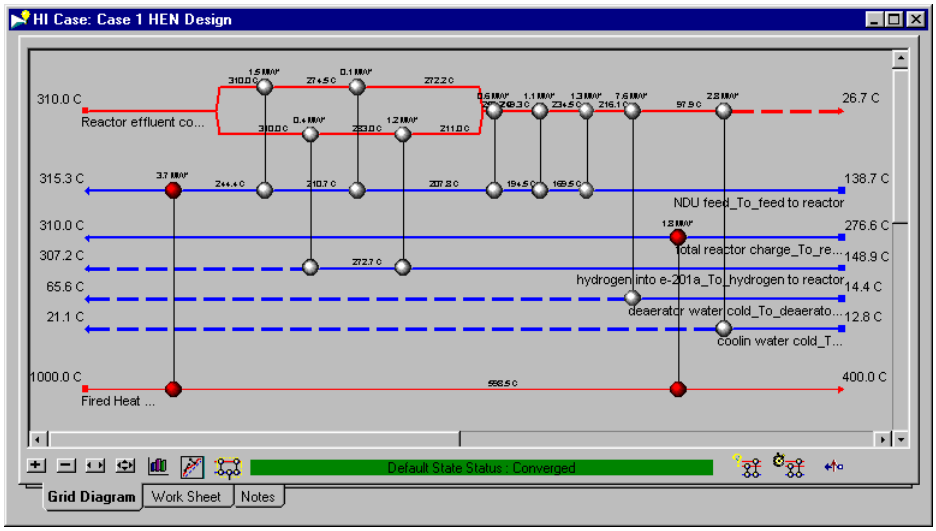
In the Operations mode, the economic parameter values are taken directly from the specified values in the Design mode. You cannot modify the economic parameter values when in Operations mode.

7.2.4 Heat Exchanger Network

Refer to **Section 6.2.7 - Grid Diagram** for more information about Grid Diagram.

The heat exchanger network (HEN) design diagram (also known as Grid Diagram) is an image that displays how individual process and utility streams are matched with one another using heat exchangers.

Figure 7.4



In Operations mode you can:

- Manipulate the Grid Diagram's appearance. Refer to the **Customize Grid Diagram View** section in **Section 6.2.7 - Grid Diagram** for more information.
- Open the Bar Chart view. Refer to **Section 7.2.6 - Bar Chart View** from the **Heat Integration** manual for more information.
- Open the Driving Force Plot view. Refer to the **Hot Driving Force Curve** and **Cold Driving Force Curve** sections in **Section 6.3.7 - Plots** for more information.
- Display the loops and paths in the Grid Diagram. Refer to **Section 6.2.9 - Loops in the Grid Diagram** and **Section 6.2.10 - Paths in the Grid Diagram** for more information.
- Controllability status of the Grid Diagram. Refer to **Section 6.4 - Controllability** for more information.

Status Bar

The status bar located at the bottom of the Grid Diagram will indicate the status of the Grid Diagram:

- If you enter the Operations mode for the first time or return the Grid Diagram to the Base Case, the status bar will be green and display the following message **Default State Status - Converged**.

  In Operations mode, the HEN is considered solved/converged even if there are some process streams that have dashed lines, and the **Target** outlet temperature for the process stream has not been reached.

Refer to the **Streams** section for the explanation on why the HEN is considered solved.

- If you have just performed multiple **What If** analyses, the status bar will display the event or schedule that was last performed.

  The status bar will be green in colour and also display **Converged** if the calculations (based on the changes made by the analysis) did converge.

Figure 7.5

The status bar will be red in colour and also display **Not Converged** if the calculations (based on the changes made by the analysis) did not converge.

Figure 7.6

- If you changed the task or event in the last performed **What If** analysis, the status bar will be yellow in colour, display the event or schedule that was last performed and the message **Not Executed**.

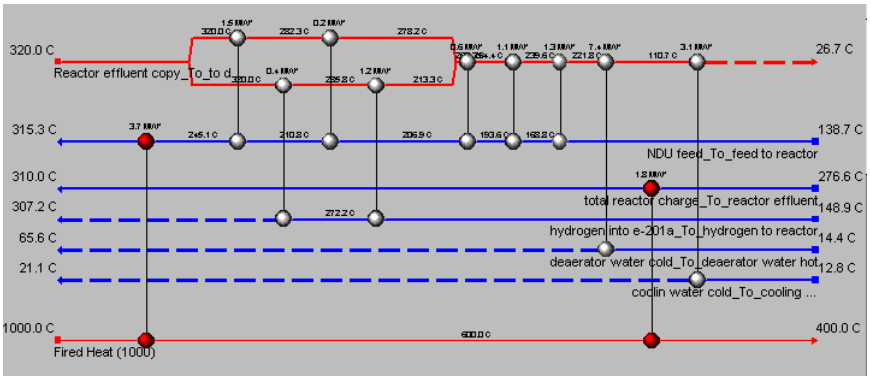
Figure 7.7

A typical HEN will contain four to five objects: process streams, utility streams, heat exchangers, and splitters-mixers.

Streams

You may notice that the process streams that have no heat transfer to or from any utility stream may not reach their Target outlet temperature. These process streams are represented by dashed lines.

Figure 7.8



The process streams exchanging heat with the utility streams are assumed to reach the Target outlet temperature because the utility streams flow rates can be varied to overcome any fouling in the exchanger or temperature fluctuations from the process streams.

So the HEN is considered converged/solved, because the system does not expect to reach the Target outlet temperature. In the *real* world, factors like fouling will reduce the heat transfer efficiency of the heat exchangers, so the calculated outlet temperature is expected to fall short from the Target outlet temperature. The Target outlet temperature is the *ideal* temperature.

Heat Exchangers

Similar to the Design mode, the Grid Diagram in Operation mode contains two types of heat exchangers: process-to-process and utility.

Process-to-Process Exchangers

Refer to the **Heat Exchangers** section in **Section 6.2.7 - Grid Diagram** for more information.

The process-process heat exchangers on the HEN appear as grey coloured discs. Each disc lays on top of the process stream that flows through the exchanger.

Utility Exchangers

Refer to the **Heat Exchangers** section in **Section 6.2.7 - Grid Diagram** for more information.

The utility exchangers on the HEN appear as red or blue coloured discs. Once disc is laid on top of the process stream that flows through the exchanger, and the other disc is laid on top of the utility stream that flows through the exchanger. Red discs indicates heaters and blue discs indicates coolers.

Area and Number of Shells in Series

Refer to **Section 3.1.1 - Entering Operations Mode** from the **Heat Integration** manual for more information about entering Operations mode.

In Operations Mode the areas of the heat exchangers are fixed. The value for the area is taken from the calculated/specified value in the Design mode. You can modify these values when entering Operations Mode.

The number of heat exchanger shells in series is another parameter fixed in operations mode and its value is calculated in the Design mode. You also can input this value when entering Operations Mode.

For heat exchangers defined as Fired Heaters no geometric parameters are considered. Refer to Section 6.2.6 - Economic Parameters for more information about Fired Heaters.

Clean Overall Heat Transfer Coefficient

The clean overall heat transfer coefficient considers that there is no fouling in the surface of the heat exchanger and is composed by the heat transfer coefficient contributions from both sides.

For shell side (hot stream):

$$\frac{U \times D}{k} = 0.36 Re_s^{0.55} \times Pr^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14} \quad (7.1)$$

Reynolds Number:

$$Re_s = \frac{D \times G_s}{\mu} \quad (7.2)$$

Shell side mass velocity:

$$G_s = \rho \times \nu = \frac{M_s}{L_{bc} \times (L_{tp} - D_t) \times (D_s / L_{tp})} \quad (7.3)$$

Prandtl Number:

$$Pr = \frac{Cp \times \mu}{k} \quad (7.4)$$

Assume:

$$\left(\frac{\mu}{\mu_w}\right)^{0.14} = 1 \quad (7.5)$$

where: U = *the heat transfer coefficient*

D = *the flow area diameter*

k = *the thermal conductivity*

ρ = *the stream density*

ν = *the stream velocity*

M_s = *the mass flow of the stream in the shell*

L_{bc} = *the baffle spacing*

L_{tp} = *the tube pitch*

D_t = *the outer tube diameter*

D_s = *the shell diameter*

μ = *the stream viscosity*

You can modify the shell diameter when entering the Operations mode. Refer to **Section 3.1.1 - Entering Operations Mode** from the **Heat Integration** manual for more information.

Cp = the effective specific heat

For tube side (cold stream):

$$\frac{U \times D}{k} = 0.023 Re_t^{0.80} \times Pr^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14} \quad (7.6)$$

Reynolds Number:

$$Re_t = \frac{D \times G_t}{\mu} \quad (7.7)$$

Tube side mass velocity:

$$G_t = \rho \times v = \frac{M_t}{(\pi \times D^2/4) \times (N_t/N_{tpass})} \quad (7.8)$$

Prandtl Number:

$$Pr = \frac{Cp \times \mu}{k} \quad (7.9)$$

Assume:

$$\left(\frac{\mu}{\mu_w}\right)^{0.14} = 1 \quad (7.10)$$

where: M_t *= the mass flow of the stream in the tubes*

N_t *= the number of tubes*

N_{tpass} *= the number of tube passes*

You can modify the number of tubes and tube passes when entering the Operations mode. Refer to **Section 3.1.1 - Entering Operations Mode** from the **Heat Integration** manual for more information.

Observed Overall Heat Transfer Coefficient

Refer to **Section 3.1.1 - Entering Operations Mode** from the **Heat Integration** manual for more information about entering Operations mode.

You can input values for the observed overall heat transfer coefficient when entering Operations Mode to account for the existing heat exchanger fouling conditions.

By default clean overall heat transfer coefficients are provided (i.e., HX-Net considers that all exchangers are clean when entering Operations Mode).

- For the purpose of studying single events that occur at a point in time, the current existing values are necessary. Refer to **Section 7.3 - What If Analysis** for more information.
- For the purpose of studying trends that occur in a certain period of time, the starting point assumes all heat exchangers are clean. Refer to **Section 7.4 - Trend Analysis** for more information.

Heat Exchanger Fouling

Based on the calculated overall clean heat transfer coefficients and the user supplied observed overall heat transfer coefficient, the dirt resistance (r_d) that measures the amount of fouling existing in a given heat exchanger is:

$$r_d = \frac{1}{U_{obs}} - \frac{1}{U_{clean}} \tag{7.11}$$

where: U_{obs} = *the heat transfer coefficient based on the specified* ***observed*** *variable values*

U_{clean} = *the heat transfer coefficient based on the default* ***clean*** *variable values*

During the execution of an event in What If analysis, changes in the physical properties that are used in calculating the overall clean heat transfer coefficient may occur. In this case, after updating the value of the overall clean heat transfer coefficient, a new value of the overall heat transfer coefficient for the heat exchanger is calculated using the formula by keeping the value of r_d constant.

Splitters and Mixers

Refer to the **Splitters and Mixers** section in **Section 6.2.7 - Grid Diagram** for more information.

On the HEN, a split in a process stream is always followed by a mixer to direct all the branch streams back to one main process stream. A process stream can have more than one split-mixer, and a split can have more than two branches.

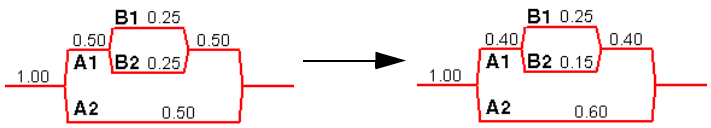
In Operations mode, you can change the flow rate between branches using the *What if analysis* features/options. However, modifying the split fraction in Operations mode will have a different effect on the flow rate, than modifying the split fraction in Design mode.

In Operations mode the percentage split between branches is fixed, while in Design mode the absolute flowrate is fixed.

The difference effects are illustrated better in the following figure:

In Design mode, consider the splits below.

Figure 7.9



First consider this setting:

- Specify **0.5** for the flow fraction in branch A1 from the first split. The flow fraction of branch A2 is automatically calculated to be 0.5.
- Specify **0.25** for the flow fraction in branch B1 from the second split. The flow fraction of branch B2 is automatically calculated to be 0.25.

You cannot specify a higher flow fraction for the second split, because the specified flow fraction applies to the overall flow rate of the process stream.

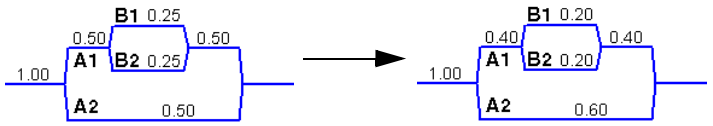
Now change the setting for the first split only:

- Specify **0.4** for the flow fraction in branch A1 from the first split. The flow fraction of branch A2 is automatically calculated to be 0.6.

The flow fraction in branch B1 is still *0.25* because it was specified, however to compensate for the decrease in flow rate from A1, the flow fraction in B2 is *0.15*.

In Operations mode, consider the splits below.

Figure 7.10



First consider this setting:

- The flow fraction in branch A1 is specified at **0.5**. The flow fraction of branch A2 is automatically calculated to be 0.5.
- The flow fraction in branch B1 is specified at **0.25**. The flow fraction of branch B2 is automatically calculated to be 0.25.

Now change the setting for the first split only:

- Specify **0.4** for the flow fraction in branch A1 from the first split. The flow fraction of branch A2 is automatically calculated to be 0.6.

The flow fraction in branch B1 and B2 is now *0.20* because the flow was originally split in half. So when the flow rate in A1 was reduced, the flow fraction of the second split maintained its *50%* split and the flow fraction in both branches was reduced by *0.05*.

7.2.5 Base Case

When you first enter the Operations mode, the calculated values and settings for the Grid Diagram are considered to be the Base Case.

HX-Net will save the values and setting of the Base Case, because the HEN is always returned to the Base Case setting before you perform a What If or Trend analysis on the HEN. So no matter how many times you perform the same and/or different analysis, the analysis is performed on the Base Case values and settings.

7.3 What If Analysis

The What If analysis is an analysis of the end result of the heat exchanger network (HEN) variable values when a single event of change is performed on the HEN. A single event contains one or more tasks.

7.3.1 Event

For information about creating events, refer to **Section 3.5.1 - Viewer Pane** from the **Heat Integration** manual.

An event is an occurrence that takes up a finite time like a day to a week. For example, the occurrence/time when a heat exchanger is being cleaned in the plant is an event.

7.3.2 Task

For information about assigning tasks, refer to **Section 3.5.1 - Viewer Pane** from the **Heat Integration** manual.

A task is the actual/physical change that takes place during an event. For example, cleaning an exchanger is a task.

As mentioned before, HX-Net contains multiple tasks, which are described below.

- Clean an exchanger. This task allows you to assign one heat exchanger to be cleaned during the event.
  To indicate that the selected exchanger is clean, you are required to enter a new overall heat transfer coefficient value. The default clean values are supplied.
- Add Area in an exchanger. This task allows you to change the heat transfer area of one heat exchanger during the event.
  To indicate that the selected exchanger's area has been modified, you are required to enter a new heat transfer area value.
- Add shell(s) in series (on each parallel pass) and rearrange tubes. This task allows you to modify the shell(s) of one heat exchanger during the event.
  To indicate that the selected exchanger's shell(s) and tubes have been modified, you are required to enter a new number of shells in series.
- Modify flowrate through a tee. This task allows you to change the flow fractions in a splitter during the event.
  To indicate that the selected splitter's flow rate has been modified, you are required to enter a new split ratio value.
- Remove an exchanger from service. This task allows you to remove one heat exchanger from the HEN during the event.
  To indicate that the selected exchanger has been removed, the heat transfer area of the exchanger has been reduced to **0 m^2**.
- Change the inlet temperature of a stream. This task allows you to change the inlet temperature of one process stream during the event.
  To indicate that the inlet temperature of the selected process stream has changed, you are required to enter the new inlet temperature value.
- Modify the flowrate of a stream. This task allows you to change the flow rate of a process stream during the event.
  To indicate the change in flow rate of the selected process stream, you are required to enter the new flow rate value.
- Study the extent of fouling in an exchanger. This task allows you to assign the amount of fouling in a heat exchanger during the event.
  To indicate that fouling has occurred for the selected exchanger, you are required to enter the fouling value of the overall heat transfer coefficient.

- Change the inlet temperature of a stream. This task allows you to change the inlet temperature of one process stream during the event.
  To indicate that the inlet temperature of the selected process stream has changed, you are required to enter the new inlet temperature value.
- Modify the flowrate of a stream. This task allows you to change the flow rate of a process stream during the event.
  To indicate the change in flow rate of the selected process stream, you are required to enter the new flow rate value.
- Modify the percentage of the flow rate for all process streams in the heat exchanger network. This task allows you to change the flow rate of all process streams during the event.
  To indicate the change in flow rate, you are required to enter the change in percentage value relative to the base case process stream flow rate. A positive value indicates the flow rates has increase. A negative value indicates the flow rates has decrease.

When an event is executed, HX-Net calculates the new HEN design's variable values based on the specified values from the tasks that occur in this event.

7.3.3 Comparing Event with Base Case

When you execute an event, the calculated variable values based on the task(s) included in the event are stored with the event. So you can compare the variable values generated by the executed event with the Base Case variable values.

This feature can be used to see how the tasks performed in your plant are affecting the overall HEN and whether the tasks performed are making the plant more or less efficient.

You can also compare the generated variable values between different events, because HX-Net will save the calculated variable results from each executed event.

If you leave the Operations mode to Design mode and enter the Operations mode again, all executed events will be erased.

7.4 Trend Analysis

An interval is a finite amount of days, weeks, months, or years.

The interval sizes are not required to be equal in Trend Analysis.

The Trend Analysis feature generates studies of the performance of a heat exchanger network (HEN) design during a given period of time. During the Trend Analysis setup process for the base case/default study, the values of observed heat transfer coefficient (HTC) can be specified for each time interval to simulate the fouling of the exchangers. Using the specified HTC values, HX-Net can calculate and plot the key HEN variable values vs. time.

The key HEN variables are:

- Utility load, which is the amount of energy/heat the exchanger transfers at each interval.
- Process stream outlet temperature, which is the calculated temperature of the process stream exiting the HEN at each interval.
- Profit index, which is the calculated amount of profit the HEN generates at each interval. The profit value is based on the specified price index of the process stream and the operating cost of the utility streams.

7.4.1 Default Study

When you first enter the Trend Analysis, you need to specify a Default Study/trend of the heat exchanger network (HEN) for comparison. The Default Study of the HEN consist of the changes in the heat exchanger's overall heat transfer coefficient values (U values) over a specified period of time. The changes in U values represent how fouling/dirt is slowly building up in the exchangers of the HEN.

HX-Net will store the U values and trend period of the Default Study, because the HEN is always returned to the Default Study setting before you perform a Trend analysis on the HEN. So no matter how many times you perform the same and/or different trend analysis, the analysis is performed on the Default Study values and settings.

7.4.2 Study

A study consist of a set of events that occur over a given period of time. The events are performed while fouling of the heat exchangers occurs over the whole analysis span. For example, the schedule to clean several exchangers in a plant over a period of weeks in a year is a study.

HX-Net provides two types of events that can occur within a study. A study can have multiple events occurring in the trend analysis and the events can overlap each other.

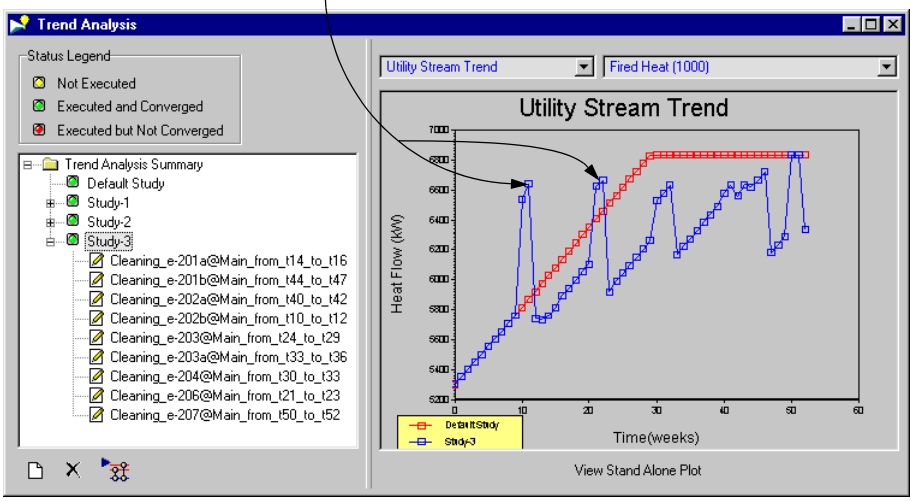
Example

Consider a plant with exchangers whose overall heat transfer coefficient (HTC) values are decreasing due to fouling. In the Default Study the exchangers are never cleaned, while in a study most of the exchangers are taken off service at some point/interval and cleaned.

The figure below displays the energy supplied by the Fired Heater (utility stream) for the Default Study and a particular study.

Figure 7.11

The peaks in the increase of energy required from the Fired Heater occur at certain intervals, because one or more heat exchangers were taken off line/service, and more energy is required from the Fired Heater to compensate for the energy lost from the out of service exchangers.



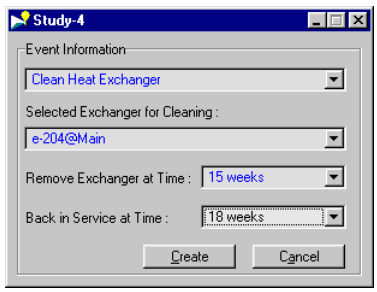
- Notice the energy required from the Fired Heater for the Default Study slowly increases until it reaches a maximum amount and cannot supply any additiona energy.
- Notice the energy required from the Fired Heater for this study is less than the maximum amount at all times. The reason is that selected heate exchangers are cleaned during certain periods of time.
  Even though the energy required increases during the cleaning, an energy decreased is observed when the cleaned exchangers are returned to service.

7.4.3 Event

An event is an occurrence that takes up a finite time like a few days or a few months. As mentioned in the previous section, there are three types of events available in the Trend Analysis feature.

- **Cleaning Heat Exchanger** event allows you to select an exchanger in the plant for cleaning. When this cleaning occurs, the selected exchanger is removed from the process for cleaning and then returned to service. You are required to specify the start and end time for the cleaning of the selected exchanger.

Figure 7.12

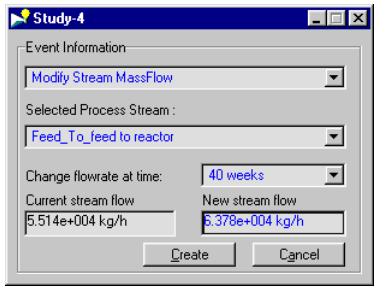


You can specify more than one flow rate change to a process stream, however, the start time of the change must be different.

So you can simulate the variation of flow rate for the process stream in the plant.

- **Modify Stream MassFlow** event allows you to vary the flow rate of a process stream in the plant. You are required to specify the starting time at which the flow rate changes and the new amount of flow rate.

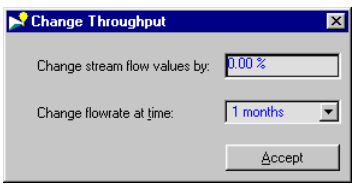
Figure 7.13



For the Change Throughput event, you can only specify one percentage value change for all the process streams.

- **Change Throughput** event allows you to vary the flow rates of all the process streams in the heat exchanger network (HEN). You are required to specify the starting time at which the flow rates change and the changed flow rates percentage value.

Figure 7.14



7.4.4 Comparing Study with Default Study

When you execute a study, the calculated key variable values based on the event(s) in the study are stored with the study. So you can compare the key variable values of executed study with the Default Study.

There are two ways to compare the data:

- **Graphical format**. The graphical format or plot of the key variable values are displayed at the study level, and the plot always displays the Default Study data points along with the selected executed study data points.
- **Tabular format**. The tabular format or table containing the key variable values are displayed at the summary level. The table will contain the variable values for the Default Study and any other studies in the Trend Analysis. For the studies that have been executed, the new calculated variable values are displayed. For the studies that have not been executed, the text **<empty>** is displayed.

If you leave the Operations mode to Design mode and enter the Operations mode again, all executed events will be erased.

8 Heat Exchanger Network Design

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8.1 Introduction

In the previous chapter, we saw how pinch analysis could be applied to examine the performance of a heat exchanger network relative to the thermodynamic optimum. A pinch analysis expert could then manually generate alternatives to structurally improve the heat exchanger network. The operation that allows you to perform the previous mentioned tasks is called the Heat Integration Project (HI Project) operation.

This chapter introduces techniques to systematically compare different alternatives generated by the expert. It also shows how HX-Net can recommend alternatives that could be very useful for the non-expert.

This chapter will describe the framework and the functionality available within HX-Net that will allow you to generate several new and retrofitted heat exchange networks (HENs). This program allows you to manually generate and compare HENs. As well, it contains several useful automated procedures.

8.2 Basic Terminology

The following sections explain the terminology and interface features that allow you to generate multiple new and retrofitted heat exchanger networks (HENs) for a system.

8.2.1 Overview

The Heat Integration Project (HI Project) view is the interface for the HI Project operation.

For more information about project view, refer to **Section 2.3.5 - Project View** in the **User Guide**.

The HI Project view contains the following:

- **Three levels**: Project, Scenario, and Design.
  The HI Project operation can contain one project level. The project level can contain multiple scenario levels, and the scenario level can contain multiple design levels.
- **Three panes**: Viewer, Main, and Worksheet.
  The Viewer pane is used to navigate from level to level, so the pane remains the same at all three levels. The information/objects in the Main and Worksheet panes vary depending on which level is selected.

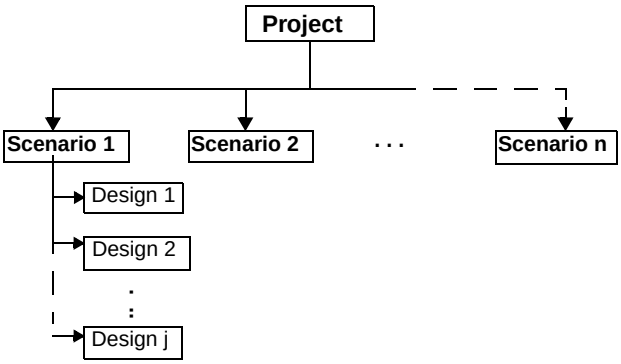
8.2.2 Heat Integration Levels and Panes

As mentioned in the previous section, the HI Project operation contains three levels. The following sections will describe each level in detail.

Project Level

At the project level, you define what you want to design. For example, you can design a heat exchanger network for a Benzene production process at a particular site, which then becomes a project. Under the project, there can be numerous scenarios.

Figure 8.1



The information at the project level will not completely specify the problem. It contains only the most general description of the problem set being examined.

Scenario Level

The scenario level contains the assumptions made to complete the information required to generate a design. For example, a Benzene process may operate at four different production rates: summer, fall, winter, and spring. Each production rate contains different process stream requirements and is referred to as a scenario in HX-Net. HX-Net lets you create and compare different designs within each scenario.

For more information about the process and utility stream data, economic data, and forbidden match, refer to **Chapter 6 - Heat Integration - Pinch Analysis**.

The Process Stream data, Utility Stream data, Economic data, and Forbidden Match data reside at the scenario level.

Design Level

Operating under a specific set of assumptions defined at the scenario level, you can create multiple heat exchanger network designs within each scenario using the operations and tools at the design level.

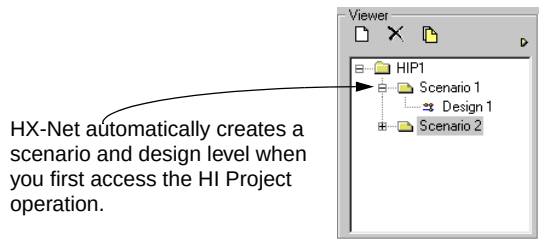
The information regarding heat exchangers and how they are connected to form a network resides at the design level.

Viewer Pane

The information/objects in the Viewer pane remain the same at all three different levels.

The Viewer pane contains a tree browser which allows you to access, create, clone, and delete scenario and design levels within a HI Project view.

Figure 8.2



Main Pane

The information and objects displayed on the Main pane depend on the active level:

- At the Project level, this pane allows you to change the name of the project level/HI Project view, and specify the name of the author/ engineer and general information about the heat transfer system being analyzed.
- At the Scenario level, this pane displays one of four different plots: Composite Curves, Grand Composite Curve, Alpha Plot, and General Plot. These plots are used to assist you in designing the heat exchanger network.
- At the Design level, this pane contains the Grid Diagram and a set of tools to manipulate or create a heat exchanger network design.

Refer to **Section 6.3.7 - Plots** for more information.

Refer to **Section 6.2.7 - Grid Diagram** for more information.

Worksheet Pane

The information and objects displayed on the Worksheet pane depend on the active level:

- At the Project level, this pane allows you to add notes to the HI Project operation. HX-Net also automatically saves the date of when the note was last modified.
- At the Scenario level, this pane allows you to enter the required information to design a heat exchanger network (HEN). This pane also displays the calculated target values and summary information of the designs within the active scenario level.
- At the Design level, this pane displays detailed information about the active HEN design and modification logs. This pane also allows you to configure or modify the HEN design.

Summary Matrix

The following table summarizes the general layout of each level of the main HI Project view.

	View Pane	Main Pane	Worksheet Pane
Project Level	Tree	General project information	Project notes
Scenario Level	Tree	Graph types: • Composite Curve • Grand Composite Curve • Alpha Plot • General Plot	Data tab: • Process Streams • Utility Streams • Economics Targets tab: • Summary • Utility Targets • Plots/Tables Range Targets tab: • Plots • Table Designs tab Options tab Notes tab
Design Level	Tree	Grid diagram	Performance tab: • Summary • Heat Exchangers • Utilities Worksheet tab Heat Exchangers tab Targets tab Notes tab: • Notes • Modification Log

8.2.3 Project Level

The following Project level procedures can be done within the Viewer Pane. Refer to the **Viewer Pane** section.

Creating a Scenario

To create a new scenario:

1. In the Viewer pane, select **HIP1** or the project level.
2. Do one of the following:
   - Click the **Add** icon.
   - Right-click in the Viewer group, and select the **Add Scenario** command from the Object Inspect menu.

Add icon

3. The Add Scenario view appears.

Figure 8.3

4. Enter a scenario name in the **Name** field, then press ENTER.

The new scenario will appear in the Viewer group.

Creating a Design

To create a new design:

1. In the Viewer group, select the **Scenario** name that will contain the new design level you want to add.
2. Do one of the following:
   - Click the **Add** icon.
   - Right-click in the Viewer group, and select the **Add Design** command from the Object Inspect menu.

Add icon

3. The Add Design view appears.

Figure 8.4

4. Enter a design name in the **Name** field, then press ENTER.

The new design will appear in the Viewer group under the selected scenario level.

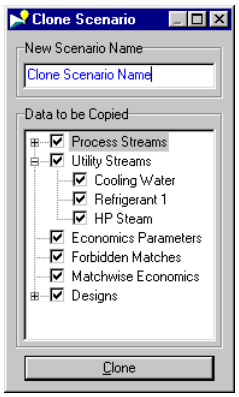
Cloning a Scenario

To clone an existing scenario:

1. In the Viewer group, select the scenario you want to clone.
2. Do one of the following:
   - Click the **Clone** icon.
   - Right-click in the Viewer group, and select the **Clone Scenario** from the Object Inspect menu.
3. The Clone Scenario view appears.

Clone icon

Figure 8.5



4. Enter a name for the cloned scenario in the **New Scenario Name** field, then press ENTER.
5. Select the data you want to copy by checking or unchecking the checkboxes in the Data to be Copied group.
6. Click the **Clone** button.

Click the **+** and **-** icons to expand or shorten the list of data in the Data to be Copied group.

The cloned scenario will appear in the Viewer group.

Cloning a Design

To clone an existing design:

1. In the Viewer group, select the design you want to clone.
2. Do one of the following:
   - Click the **Clone** icon.
   - Right-click in the Viewer group, and select the **Clone Design** from the Object Inspect menu.
3. The Clone Design view appears.

Clone icon

Figure 8.6

4. Enter a design name for the cloned design in the **Name** field, then press ENTER.

The cloned design will appear in the Viewer group under the scenario level that contained the original design.

Removing a Scenario or Design

To remove an existing scenario or design:

1. Select the scenario or design you want to delete in the Viewer group.
2. Do one of the following:
   - Click the **Delete** icon.
   - Right-click in the Viewer group, and select **Delete Scenario** or **Delete Design** command from the Object Inspect menu.
3. HX-Net will ask you to confirm deletion of the scenario or design before deleting the selected level.
   - Click the **Yes** button to delete the selected level.
   - Click the **No** button to keep the selected level.

Delete icon

The deleted scenario or design will be removed from the Viewer group.

8.2.4 Scenario Level

The scenario level is where you enter the data required to construct a heat exchanger network (HEN). If you have different data for three different situations, you can create three scenarios to represent each situation.

Basic Information

The basic information required to build a HEN includes the following:

- The inlet temperature, outlet temperature, and MCp or enthalpy of the process stream. Refer to **Section 6.2.1 - Process Streams** for more information.
- The inlet temperature, outlet temperature, and the cost per energy of the utility stream. Refer to **Section 6.2.2 - Utility Streams** for more information.
- The economic parameters for the capital cost of the heat exchanger. Refer to **Section 6.2.6 - Economic Parameters** for more information.

You have the choice of defining your own utility, selecting one of the default utility, or selecting a modified default utility. Refer to **Section 10.2 - Utility Database View** in the **User Guide** for more information.

Aside from the basic information, you can specify/modify the heat transfer coefficient for the process and utility streams. Refer to **Section 6.2.5 - Heat Transfer Coefficient** for more information.

Target Values

For each scenario, HX-Net will take the specified basic information and calculate variable values for an ideal situation/HEN design. The ideal values of the variables are based on the pinch analysis.

Refer to **Section 6.3 - Targets** for more information about target values.

The variables considered in the pinch analysis are energy, heat transfer area, capital cost, operating cost, and minimum number of exchangers. These variables are referred to as target values.

The target values are displayed in two formats: tabular and graph. The tabular format provides a value to value comparison between your current HEN configuration and the ideal HEN configuration.

The graphical format is divided into four different types of plots:

- The **Alpha Plot** displays ideal (target) capital cost values against ideal (target) operating cost values which are calculated at different minimum approach temperatures. The designs in a scenario are displayed as points on the Alpha Plot and are always situated above the ideal curve. This allows you to compare the Designs with one another and with the target values.
- The **Grand Composite Curve** is a plot of shifted temperatures vs. the cascaded heat between each temperature interval. The grand composite curve is particularly useful for determining the placement of hot and cold utilities.
- The **Shift Composite Curve** is a graphical means to depict (or composite) all hot or cold process streams in a heat exchange network.
- The **General Plot** can be customized to display any one of eight properties along the X-axis and either the right Y-axis, left Y-axis, or both. The following table lists and describes the eight properties:

For more information on the Grand Composite Curve and the Shift Composite Curve, refer to **Section 6.3.7 - Plots**.

Property	Description
Heating	Displays the total load on the heating utilities.
Cooling	Displays the total load on the cooling utilities.
Total Area	Displays the total area of the heat exchangers in the design(s).
Units	Displays the number of heat exchangers in the design(s).
Shell	Displays the number of shells in the design(s).
Capital Cost Index	Displays the capital cost of the design(s).
Operating Cost Index	Displays the total operating costs for the design(s), which is a total of the heating and cooling costs.
Total Cost Index	Displays the total cost, which is a sum of the operating and annualized capital costs.

Design Comparison

The table is empty/blank if there are no HEN designs in the active scenario level.

At the Scenario level there is a table that contains summary information for all the HEN designs within the selected/active scenario. The table also displays the same summary information from the target values.

This table allows you to compare and select the optimum design from all the possible designs within the active scenario level.

- You can toggle between displaying only completed designs or all designs (complete and incomplete designs) in the table.
- You can also toggle between displaying the summary information in percentage values relative to the target values.

8.2.5 Design Level

The design level is where you construct the heat exchanger network (HEN). You can create and compare multiple unique designs for each scenario level.

Basic Information

As in the Scenario level, you are required to enter basic information/ data for the construction of the HEN design. In the design level, the basic information includes adding heat exchangers and splitters to the Grid Diagram. For more information about building the HEN design, refer to **Section 6.2.7 - Grid Diagram**.

Performance Evaluation

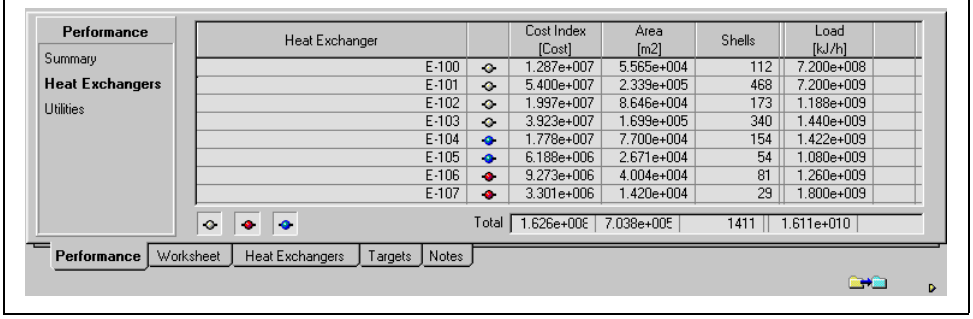
After completing the HEN design, you can compare the cost and performance of the design with the ideal design.

- The heating, cooling, operating, capital, and total cost values are displayed as well as the percentage values relative to the target values.
- The amount of energy being transferred for heating and cooling purpose in the design are displayed as well as the percentage values relative to the target values.
- The number of exchangers, number of shells, and the total heat transfer area values are displayed as well as the percentage values relative to the target values.
- The individual utility cost and load for all the utilities in the design are displayed. The percentage values of the utility load relative to the target values are also displayed.

All the information available in the HI Case operation (**Chapter 6 - Heat Integration - Pinch Analysis**) is also available in the HI Project operation, however, the HI Project operation displays the following information which does not appear in the HI Case operation:

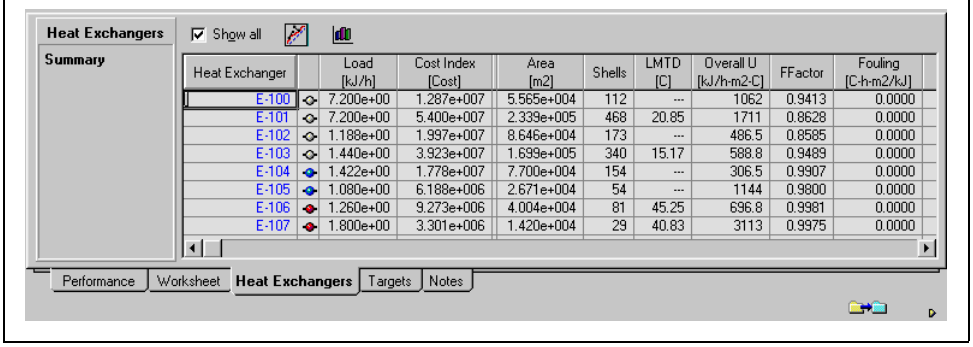
- The number of shells for each heat exchanger appears in the heat exchanger summary table.

Figure 8.7



- A table containing the detail information on all the heat exchangers appears in the HEN design.

Figure 8.8



8.2.6 Operation Modes

The HI Project operation is similar to the HI Case operation. Both operations have two modes, one for designing and the other for analyzing/simulating.

The two HI Project modes are as follows:

- **Design mode**. In this mode, you can create several designs automatically or manually. You can then compare the designs with one another, or with heat integration targets.
- **Retrofit mode**. In this mode, you can generate new and retrofitted HEN designs to compare with an existing base HEN design. The comparisons are made in terms of additional investment and operating cost savings.

Design Mode vs. Retrofit Mode

When a scenario is switched from Design mode to Retrofit mode the following changes occur:

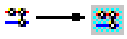
Design mode

Retrofit mode

- The Retrofit mode scenario contains only one design from the Design mode scenario. This design is known as the base case. It is recommended that you do not change anything in the base case, as this design will be compared with the retrofitted design to see what changes the retrofit feature has made.
- The **Folder** icon in the Main pane and Viewer pane changes colour from yellow to blue.
- The **Area vs. Heat Demand** plot is added to the Main pane. This plot displays the heating requirements for the simulation base case and the different retrofit designs using the corresponding total heat area.
- The **Investment vs. Savings** plot is added to the Main pane. This plot displays the annual savings obtained in each of the retrofit designs when the corresponding investment is placed. A two-year payback line is added for reference.
- The **Investment vs. Payback** plot is added to the Main pane. This plot displays the payback of the investment for the simulated base case and the different retrofit designs.
- The variable values from the base case is displayed along with the target values in the **Targets** tab, **Summary** page.
- When comparing designs in the scenario, the retrofitted designs are compared to the base case design in the **Designs** tab.
- The **Subsets** tab is removed from the Worksheet pane.
- The **Data Extraction from Simulation** icon is no longer available.

Refer to the **Comparing Designs** section from **Section 8.3.2 - Automated Retrofit Capabilities** for more information about the changes in the Designs tab.

Unlock Retrofit Mode icon



Design vs. Base Case icons

- The **Enter Retrofit Mode** icon has been replaced with the **Unlock Retrofit Mode** icon.

When a design is switched from Design mode to Retrofit mode the following changes occur:

- The imported/selected existing design is known as the base case and the icon beside the design's name turns light blue in colour.
- The Zoom option icons in the Main pane turn light blue in colour.
- The five Retrofit option icons are made available in the Grid Diagram Palette. Refer to the **Five Types of Retrofit Options** section from **Section 8.3.2 - Automated Retrofit Capabilities** for more information about the retrofit options.
- The options to place limits on the heat transfer area and spare heat transfer area of the exchangers in the HEN design are made available.

8.3 Automated Procedures

HX-Net contains two features that automatically generate or modify the heat exchanger network (HEN) to an optimum design.

- The **Automatic Recommend Designs** (ARD) feature generates an optimum HEN based on the specified data/basic information.
- The **Automatic Retrofit** feature makes small modifications on an existing HEN to improve the efficiency of the existing design.

The operation mode can impact automated procedures. Refer to **Section 8.2.6 - Operation Modes** for more information.

The following sections explain the automated features in detail.

8.3.1 Automated New Designs

The Automatic Recommend Designs (ARD) feature builds an optimum HEN design based on the given basic information. The basic information includes the following:

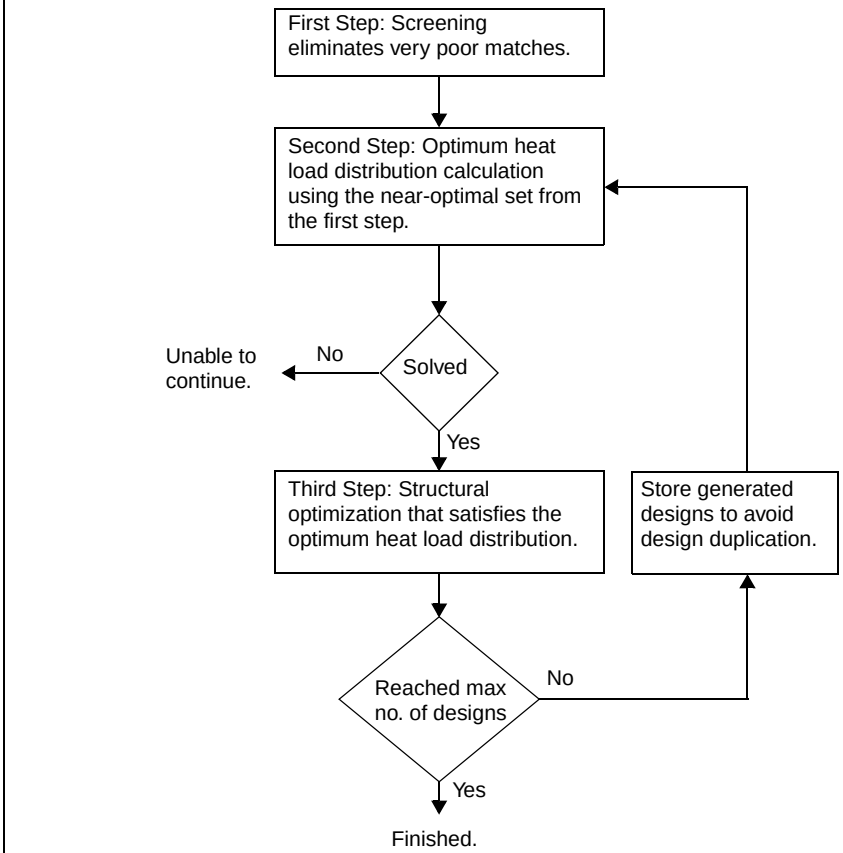
- Process and utility stream supply and target temperatures.
- Process stream's heat loads.
- Temperature-dependent specific heat and heat transfer coefficients for each stream.
- Operating cost per unit heat load of each utility.
- Capital cost of placing a heat exchanger on each possible match.

Once all the above information/assumptions has been supplied, you can activate the ARD feature. The feature generates optimum designs using a three-step approach.

Theory and Algorithm

This section describes in detail the three-step procedure the Automatic Recommend Design feature uses to generate the optimum HEN designs.

Figure 8.9



First Step

In the first step, a LP (linear programming) model is set up to simultaneously optimize heat exchange area and heat load for each utility. The purpose of this optimization is to eliminate very poor matches.

Second Step

The LP model in the first step does not account for the number of heat exchange units in the objective function. This issue is addressed in the second step using a mixed integer linear model (MILP1), which simultaneously optimizes the model for heat exchanger units, heat exchanger area and heat loads on each utility.

1. In the model, heat exchanger matches are placed between each hot stream in each temperature interval and all cold streams in all subsequent temperature intervals.
2. The objective function is linear and it minimizes the total annual cost of the HEN subject to heat balance constraints.
3. The temperature intervals are generated with a temperature shift just greater than zero. Each temperature interval is small enough that HX-Net can linearize the log-mean temperature difference on each match while maintaining the accuracy.
4. Flow rate continuity constraints are written on utility streams so that HX-Net can account for non-point utilities.

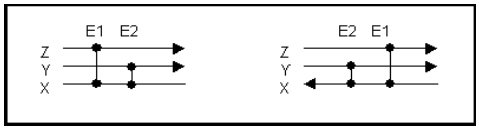
At this stage, the optimal heat load and approach temperature on each hot-cold stream match pair (i.e., the optimal heat load distribution) are known, but the physical positioning of the exchangers are unknown.

The solution provides the heat loads on each utility in the case of multiple hot and cold utilities, and the heat load on every match pair. The match pairs with zero heat load are non-optimal matches and no heat exchange should be performed between these matches. The solution of the model also provides us with an optimal approach temperature for each match pair that exists.

The positions of matches E1 and E2 is still undetermined. A detail description of this model is presented in Shethna et al (2000).[140]

For example, from the solution of the MILP1, HX-Net determines that it is optimal to match a hot stream X with cold streams Y and Z. The solution, however, does not clarify the position of the exchangers between streams X and Y and streams X and Z as shown in the following figure.

Figure 8.10



The optimal heat load distribution of match pairs between X and Y (E1) and X and Z (E2) is known, but the positions of pairs on the network is unknown after solution of first model.

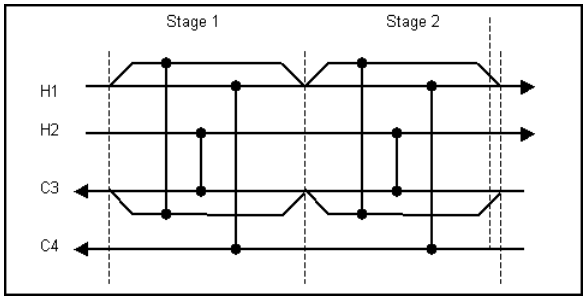
Third Step

For the example shown in **Figure 8.10**, the solution model (MILP2) will be able to find one of the two heat exchanger networks.

Another mixed-integer-linear model (MILP2) is formulated that identifies a heat exchanger network that satisfies the optimal heat load distribution obtained from the solution of the first model.

1. In this model, HX-Net formulate a superstructure in a manner similar to that proposed by Yee and Grossman (1990)[176] as shown in the figure below.

Figure 8.11



Superstructure comprises of stages wherein each stage an exchanger is placed for each match pair that exists in the solution of MILP1.

2. In the superstructure, each stream is divided into a given number of stages.

3. In each stage an exchanger is placed on each match pair that exists in the solution of MILP1. A mixed-integer-linear-model (MILP2) is formulated that models the superstructure described above.
4. The objective function used is to minimize the deviation of the heat load distribution of the actual heat exchanger network from the heat load distribution recommended from MILP1. The underlying assumption here is that any heat exchanger network obtained from the solution of MILP2 that matches the heat load distribution obtained from MILP1 is near-optimal.
5. In the optimization formulation, a heat balance and a temperature difference constraint is written across each heat exchanger. Also, more sophisticated constraints are written on each stream in each stage to account for the segmentation of streams.

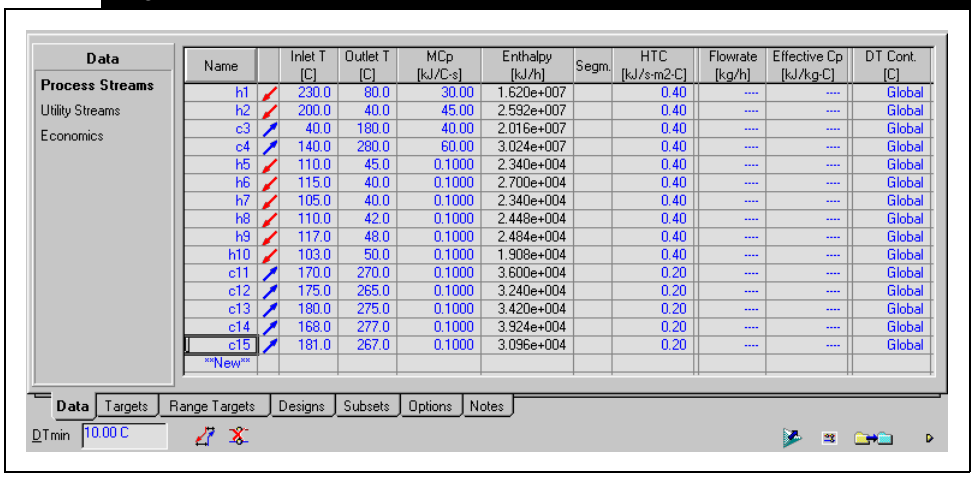
On solving this model, HX-Net obtains the heat load on each of the heat exchangers in these stages. Those exchangers with zero heat load will be eliminated.

Example

Consider the basic information provided in the following figures:

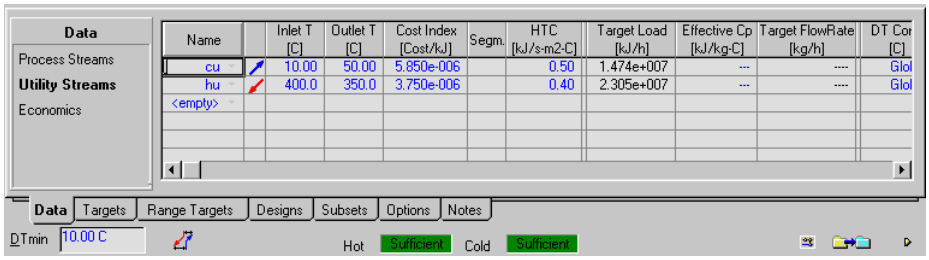
- the process stream

Figure 8.12



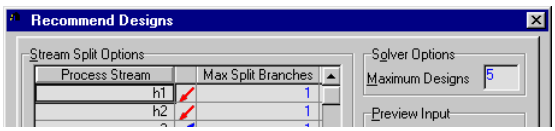
- the utility stream

Figure 8.13



- the maximum number of possible branches for all the process streams and the number of recommended designs to be kept

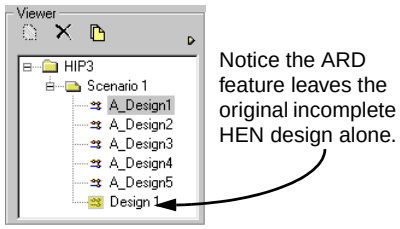
Figure 8.14



The optimum designs are automatically named "A_Design" followed by an integer number (whose value increases by one for each subsequent design).

Based on the previous information, HX-Net will generate five optimum designs.

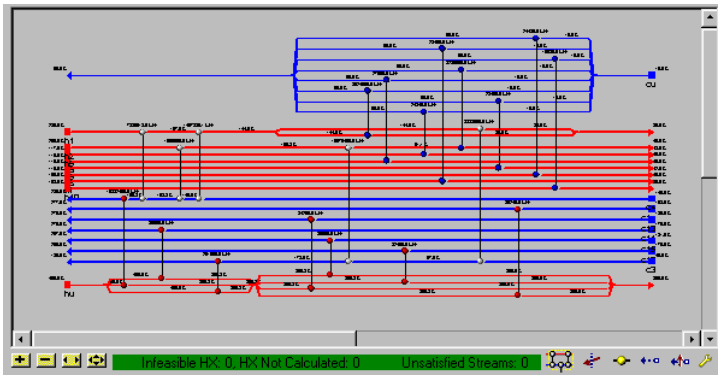
Figure 8.15



The utilities stream can contain any number of branches while the process stream has been limited to one or no branches as specified in the Recommend Designs view.

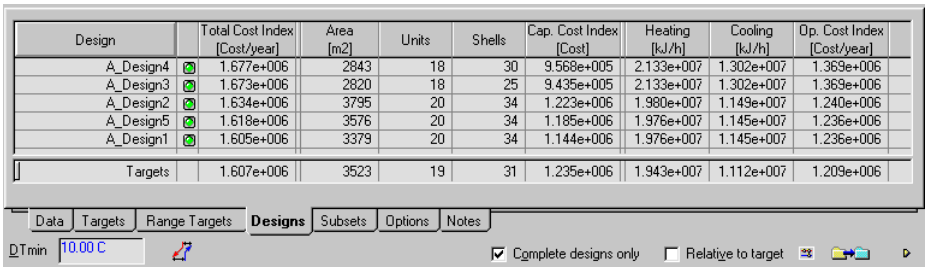
The figure below displays a HEN design generated by the ARD feature:

Figure 8.16



You can compare the generated optimum designs and select the one most appropriate, as shown in the figure below:

Figure 8.17



Design	Total Cost Index [Cost/year]	Area [m2]	Units	Shells	Cap. Cost Index [Cost]	Heating [kJ/h]	Cooling [kJ/h]	Op. Cost Index [Cost/year]
A_Design4	1.677e+006	2843	18	30	9.568e+005	2.133e+007	1.302e+007	1.369e+006
A_Design3	1.673e+006	2820	18	25	9.435e+005	2.133e+007	1.302e+007	1.369e+006
A_Design2	1.634e+006	3795	20	34	1.223e+006	1.980e+007	1.149e+007	1.240e+006
A_Design5	1.618e+006	3576	20	34	1.185e+006	1.976e+007	1.145e+007	1.236e+006
A_Design1	1.605e+006	3379	20	34	1.144e+006	1.976e+007	1.145e+007	1.236e+006
Targets	1.607e+006	3523	19	31	1.235e+006	1.943e+007	1.112e+007	1.209e+006

8.3.2 Automated Retrofit Capabilities

The Automatic Retrofit feature allows you to select different types of modifications to improve the efficiency of an existing heat exchanger network (HEN).

The following sections discuss:

- the theory and algorithm behind the Automatic Retrofit feature
- the typical procedure used to retrofit an existing HEN
- the different terminology used in HX-Net to represent different retrofitted designs
- the different ways to compare the retrofitted designs with the existing HEN
- the types of constraints available to narrow the search for a feasible retrofit design

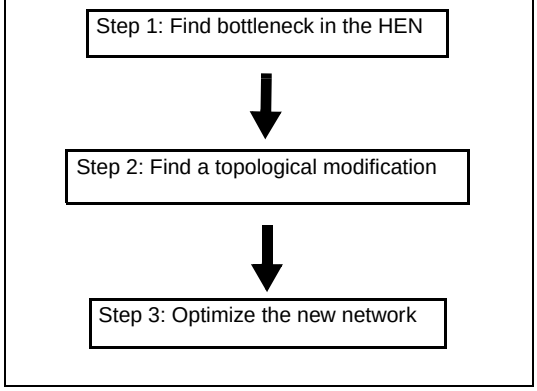
Theory and Algorithm

The two most often used methods in a HEN retrofit are the pinch design method and the mathematical programming method. The pinch method is more time consuming and results are based on the experience and judgment of the designer, but offers more “hands-on” approach to the problem. While the mathematical programming method is less time consuming and has a detailed approach to finding the solution, it requires less user interaction. The Automatic Retrofit feature uses a combination of both methods.

The Automatic Retrofit feature performs the retrofit using a two-stage process. The first stage locates the bottleneck(s) in the system. The second stage removes bottleneck(s) by making modifications to the system. Capital Energy trade-off is also performed in the second stage.

The figure below shows a simplified view of the HEN Retrofit Algorithm:

Figure 8.18



Finding the Bottleneck in the Heat Exchanger Network

For more information on bottlenecks and retrofit, refer to the report written by Asante & Zhu (1997)[11].

The loops and paths in an existing HEN system are used to reduce energy consumption. There will come a point when the scope of energy reduction cannot go any further due to the original HEN set up. This limitation causes bottlenecks in the system. HX-Net performs this stage automatically.

Removing the Bottleneck from the Heat Exchanger Network

The second stage of the Automatic Retrofit process is to remove these bottlenecks and optimize the energy consumption. A linear mathematical model is applied to remove the bottleneck. This is done with one of the following four types of modifications:

- Increasing the heat transfer area of an existing exchanger.
- Moving one end of an existing exchanger to a different location on the same stream, or moving one end of an existing exchanger to a different stream.
- Moving both ends of an existing exchanger to different locations on the same streams or different streams.
- Adding a new heat exchanger in the heat exchanger network (HEN).

After removing the bottlenecks, the Automatic Retrofit process optimizes the network energy and area. This requires a non-linear model to be solved. Automatic Retrofit minimizes the new area required, not the total area of the network.

The Automatic Retrofit feature also offers a fifth modification option: modifying the utility heat exchanger. This option involves adding or repiping coolers and heaters to lower cost utilities that are available but have not been used.

The Automatic Retrofit feature is set up so that you can choose which type of modification to apply to the HEN and how many times the modification is applied on the system. The design engineer can also specify constraints such as a limit on additional area in heat exchangers, existing spare area on heat exchangers, and heat exchangers that can't be modified. Each time a modification is applied, the retrofit goes through the entire two-stage process.

The end results will depend on the selected design and which type of modification was chosen. This step-by-step modification and the ability to choose the type of modification allows you to more closely control the HEN retrofit process.

The types of modifications are placed in a recommended step sequence as follows: Utility, Resequence, Repiping, New Heat Exchanger, and Heat Transfer Area. The recommend modifications are arranged so that the modifications that require minimal changes to the existing network are performed initially.

Retrofit Procedure

The following is a summary of the typical procedure used for retrofitting an existing heat exchanger network:

1. Access an existing and complete heat exchanger network (HEN). There are two methods in obtaining the HEN:
   - Extract from HYSYS simulation an existing plant using the **Data Extraction** feature. HX-Net will extract the relevant data from the entire HYSYS simulation and generate a complete HEN design of the existing plant.
   - Build the existing HEN using the HI Project operation by creating a scenario where you enter all the basic information for the HEN system and creating a design where you enter the basic information to match the existing HEN design.

Refer to **Section 6.5 - Data Extraction** for more information.

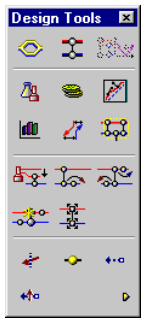
Enter Retrofit Mode icon

2. Enter the Retrofit mode by clicking the **Enter Retrofit Mode** icon. Refer to **Section 5.1.1 - Entering the Retrofit Mode** in the **Heat Integration** manual for more information.
3. In the Retrofit mode, the retrofit scenario will contain a base case/ existing HEN design. Select the base case design.
   The base case design is the original/existing design to which all retrofit modifications are applied.

Open Palette View icon

4. Access the five retrofitting options available in the Grid Diagram palette by clicking the **Open Palette View** icon.
5. Select the retrofit option you want to perform on the base case by clicking the appropriate retrofit option icon in the Grid Diagram palette.

Figure 8.19

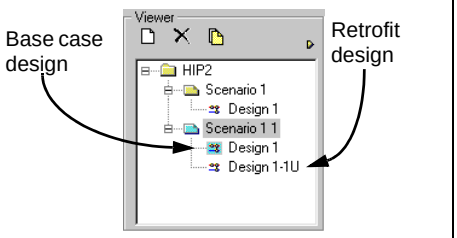


Refer to the **Five Types of Retrofit Options** section for more information.

Refer to **Retrofit Design Terminology** for more information about retrofit designs.

6. If the retrofit option is performed successfully, a new design based on the retrofit modification will appear under the retrofit scenario.

Figure 8.20



Refer to the **Comparing Designs** section for more information.

7. After making the retrofit modifications required, you can go to the retrofit scenario level and compare the base case design with the retrofit design in the **Designs** tab.

Five Types of Retrofit Options

As mentioned in the **Theory and Algorithm** section, there are five types of retrofit options:

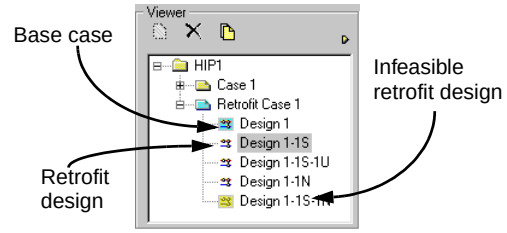
- **Modify utility heat exchanger: changes** the utility connected to the coolers or heaters to reduce the operating cost of the HEN.
- **Resequence a heat exchanger**: changes the cold or hot stream flowing through the heat exchanger for more efficient heat transfer. With more efficient heat transfer the heat transfer area can be reduced and/or the amount of duty required from the utility can be reduced, thus reducing capital cost and/or operating cost of the exchangers.
- **Repiping a heat exchanger**: changes both the cold and hot streams flowing through the heat exchanger for more efficient heat transfer to reduce the heat transfer area and/or the amount of duty required from the utilities, therefore reducing the capital cost and/or operating cost of the exchangers.
- **Add a heat exchanger**: adds another heat exchanger to the HEN design to increase the heat transfer efficiency between the process streams and/or utility streams. More efficient heat transfer will reduce the amount of duty required by the utilities and reduce the operating cost.
- **Add area**: increases the heat transfer area in heat exchanger to increase the heat transfer efficiency. More efficient heat transfer will reduce the amount of duty required by the utilities and the operating cost.

Retrofit Design Terminology

New designs generated by the retrofit option will automatically be named with the original design's name and an extension to indicate the type of retrofit performed on the new design.

For example, if you perform an Add Exchanger retrofit option on a base case design called Design 1, a retrofit design will appear under the retrofit scenario with the following name: Design 1-1N. This appears in the figure below.

Figure 8.21



The following is a list of all the extensions used to designate the type of retrofit option performed on the design:

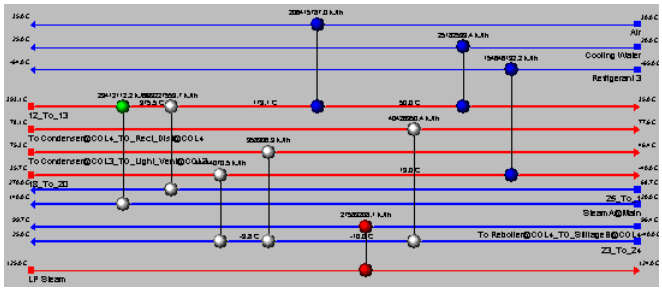
Extension	Description
-N	Indicates that a new heat exchanger has been placed.
-U	Indicates that a utility connection has been changed
-S	Indicates that a heat exchanger was resequenced.
-P	Indicates that a heat exchanger was repiped.
-A	Indicates that the heat transfer area of a heat exchanger has been modified.

You cannot perform two retrofit options at the same time to generate a retrofit design containing both options.

You can only perform only one retrofit option at a time. For example, if you perform the Resequenced retrofit option on a base case, a retrofit design (containing only a heat exchanger with modified cold or hot stream connection) is added under the retrofit scenario. As shown in the Figure 8.21, the retrofit design is named Design 1-1S.

The Grid Diagram of the retrofit design will also contain one heat exchanger (green in colour) to indicate the heat transfer area has been modified for the heat exchanger.

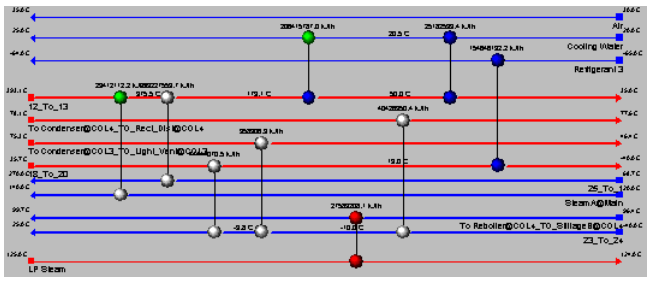
Figure 8.22



For a design to contain more than one retrofit option, you must perform the next retrofit option on the design that has been previously retrofitted. HX-Net will generate a new retrofit design based on the selected design and selected retrofit option.

For example, if the Modify Utility retrofit option was performed on the Resequenced retrofit design (i.e., Design 1-1S from **Figure 8.21**), the result is a new retrofit design added to the retrofit scenario with the following name Design 1-1S-1U. The Design 1-1S-1U contains an exchanger with modified hot or cold stream connection and an exchanger with modified utility connection. The retrofit modifications are indicated by the green heat exchanger icons in the Grid Diagram.

Figure 8.23



If the retrofit option causes one or more heat exchangers to become infeasible, the icon beside the retrofit design will be yellow in colour as shown in Figure 8.21. The Grid Diagram of the infeasible retrofit design will contain yellow coloured heat exchanger(s) that indicates which exchanger(s) have become infeasible.

Comparing Designs

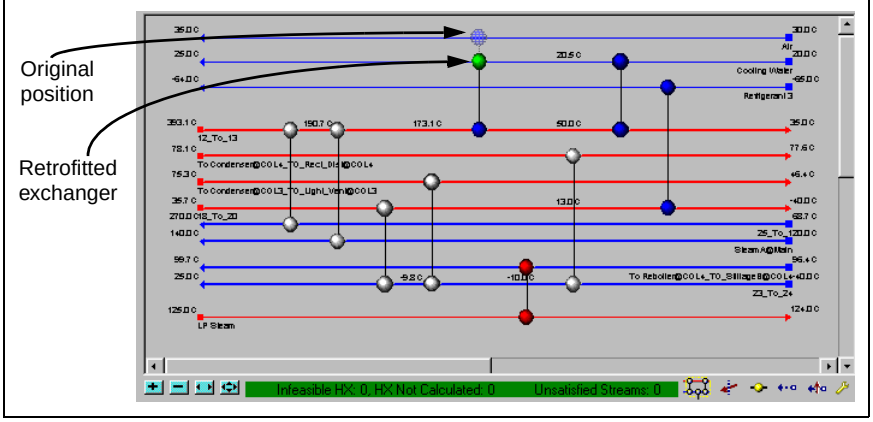
After you have finish applying the retrofit option(s) to the base case design, you can do the following:

- View in detail the changes made to the modified heat exchanger(s) in each retrofit design(s) at the design level.
- Compare the cost and/or energy savings of the retrofitted design(s) at the scenario level.

Design Level

At the design level, you can see which exchanger was modified by the retrofit option in the Main pane. The Main pane will contain the Grid Diagram and the modified exchanger will be green in colour as shown in the figure below.

Figure 8.24



The Worksheet pane of the retrofit design allows you to compare the performance differences between the selected retrofit design, base case, and/or the target.

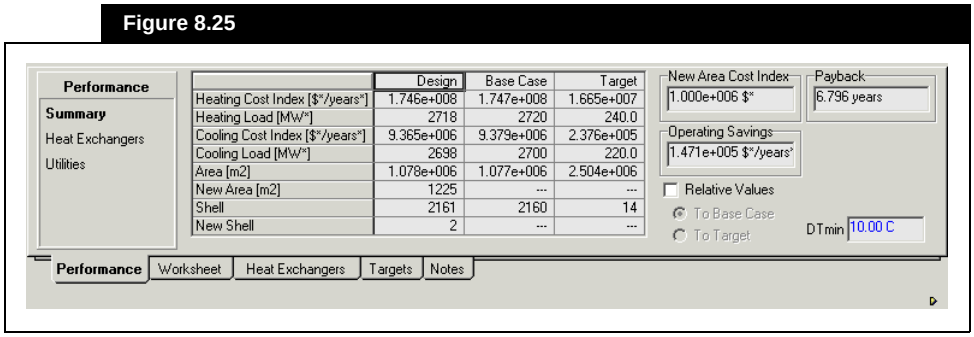
Performance Tab

The Performance tab contains summary information for the target, base case, and retrofitted design, so you can easily compare the changes made by the retrofit option. The tab is divided into three pages: Summary, Heat Exchangers, and Utilities.

Summary Page

The Summary page displays the calculated values for a number of key variables for non-base case designs, and displays them along with the base case design and the target values.

Figure 8.25



The Summary page contains a table that displays a list of variable values for the following three situation: retrofit modified design, base case, and target.

The following table lists and describes the variables displayed in the Summary table:

Variable	Description
Heating Cost Index	Displays the actual cost of the hot utilities used in the design.
Heating Load	Displays the sum of the loads on the hot utilities in the design.
Cooling Cost Index	Displays the actual cost of the cold utilities used in the design.
Cooling Load	Displays the sum of the loads on the cold utilities in the design.
Area	Displays the sum of all the heat exchanger areas in the design.
New Area	Displays the sum of all the new area used for the new design.
Shell	Displays the total number of shells used in the design.
New Shell	Displays the sum of all the new shells used for the new design.

The new area is the difference between the new design area and the base case area.

The values in the table can be displayed as percentages, relative to either the base case design or the target values. To see the values as percentage, do the following:

1. Check the **Relative Values** checkbox.
2. Select either the **Base Case** or **Targets** radio button.

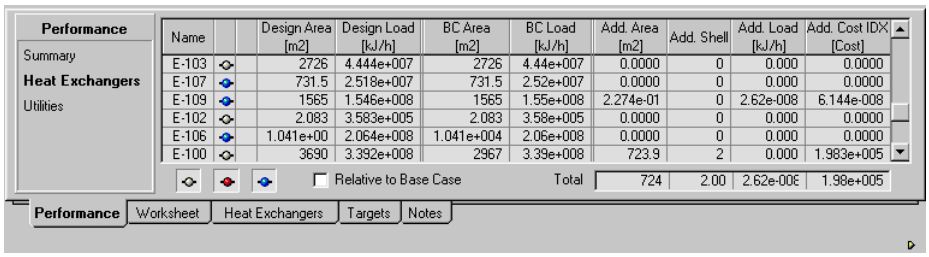
The following table lists and describes the four fields in the Summary page:

Field	Description
New Area Cost Index	Displays the cost of the new area in the design.
Payback	Displays the number of years required to recover the costs associated with the new area.
Operational Savings	Displays the savings per year associated with the reduced utility loads.
DTmin	Allows you to specify the minimum temperature difference for all the heat exchangers in the design.

Heat Exchangers Page

The Heat Exchangers page displays the values of capital cost related parameters, calculated from the heat exchangers placed on current design.

Figure 8.26



The following table lists and describes the information available in the Heat Exchangers page:

Object	Description
Name column	The name of the heat exchanger, as defined on the Worksheet tab or in the Heat Exchanger Editor view.
Heat Exchanger Type column	Displays an icon that indicates the heat exchanger type. There are three types of heat exchangers: Process-process, Cooler, and Heater.
Status column	This column displays information about the status of the heat exchanger calculations. • **OK Status.** The specifications are OK and the heat exchanger is feasible. No icon appears. • **Partially Calculated.** There is insufficient information about the conditions to complete the calculations. Yellow icon appears. • **Under Specified**. Some of the conditions are specified and some of the conditions are not specified, for either the heat exchanger or the stream. Yellow icon appears. • **Over Specified**. There are too many conditions specified. Yellow icon appears. • **Infeasible.** The specifications provided will not make a feasible heat exchanger. Red icon appears. • **Failed to Calculate.** There was a problem with the calculations. Red icon appears.
Design Area column	The area of the heat exchanger in the current design.
Design Load column	The load of the heat exchanger in the current design.
BC Area column	The area of the same heat exchanger in the base case design.
BC Load column	The load of the same heat exchanger in the base case design.
Add. Area column	The additional heat exchanger area in the current design (extra added on to the base case design area).
Add. Shells column	The additional shells on the heat exchanger in the current design (extra added on to the base case design area).
Add. Load column	The additional load on the heat exchanger in the current design (extra added on to the base case design). The values are either zero or positive numbers.
Add. Cost IDX column	The additional capital cost associated with an additional area that has been added to the heat exchanger.
Displays Process-Process Exchangers icon	Allows you to toggle between showing or hiding the Process-Process heat exchangers data in the table.
Displays Heater icon	Allows you to toggle between showing or hiding the Heaters data in the table.
Displays Cooler icon	Allows you to toggle between showing or hiding the Coolers data in the table.

Yellow icon represents: Partially Calculated, Under Specified, and Over Specified status.

Red icon represents: Infeasible and Failed to Calculate status.

Show and Hide Process-Process Exchangers icons

Show and Hide Heaters icons

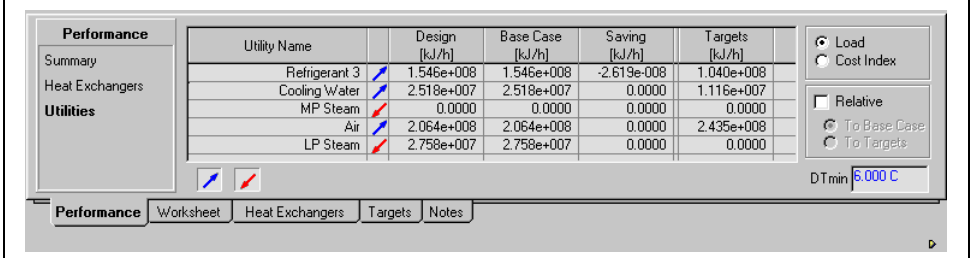
Show and Hide Coolers icons

Object	Description
Relative to Base Case checkbox	Allows you to toggle between displaying the values on the table as a percentage of the base case value or as the actual design values.
Total row	Displays the total values for the additional area, additional shells, additional load, and additional cost index.

Utilities Page

The Utilities page contains a summary of the operating costs and utility loads associated with the heat exchanger network design.

Figure 8.27



The following table lists and describes the objects available in the Utilities page:

Hot and Cold Stream icon

Object	Description
Utility Name column	Displays the name of the utility.
Utility Type column	Displays an icon that indicates the utility type.
Design column	Displays the load on the utility or the operating cost associated with the utility in the current design, depending on the radio button selection.
Base Case column	Displays the load on the utility or the operating cost associated with the utility in the base case design, depending on the radio button selection.
Saving column	Displays the load or cost savings between the current design and the base case design, depending on the radio button selection.
Targets column	Displays the target load or target operating cost associated with the utility, depending on the radio button selection.
Load radio button	When selected, allows you to display the variable information in the table in terms of load related values.
Cost Index radio button	When selected, allows you to display the variable information in the table in terms of cost related values.

Displays cold stream, hide hot stream.

Hide cold stream, displays hot stream.

The *To Base Case* and *To Targets* radio buttons are only available if the *Relative* checkbox is checked.

Object	Description
Displays Cold Utility Stream icon	Allows you to toggle between hiding or displaying the cold utility stream in the Utility Targets table. The default setting for this icon is active.
Displays Hot Utility Stream icon	Allows you to toggle between hiding or displaying the hot utility stream in the Utility Targets table. The default setting for this icon is active.
Total row	Displays the sum of the operating costs for the current design, the base case, the saving between the current design and base case, and the target values. This row is only available if the Cost Index radio button is selected.
Relative checkbox	Allows you to toggle between displaying the values in the tables as a percentage relative values or as the actual values.
To Base Case radio button	Allows you to display the values in the table as a percentage relative to the base case values.
To Targets radio button	Allows you to display the values in the table as a percentage relative to the targets values.
DTmin field	Allows you to specify the minimum temperature difference for all the heat exchangers in the design.

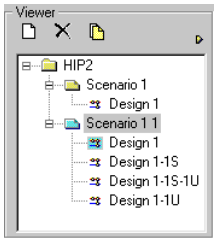
To see the values in the table as percentage, do the following:

1. Checked the **Relative Values** checkbox.
2. Select either the **Base Case** or **Targets** radio button.

Scenario Level

At the scenario level, you can compare the cost savings obtained through the retrofit option(s).

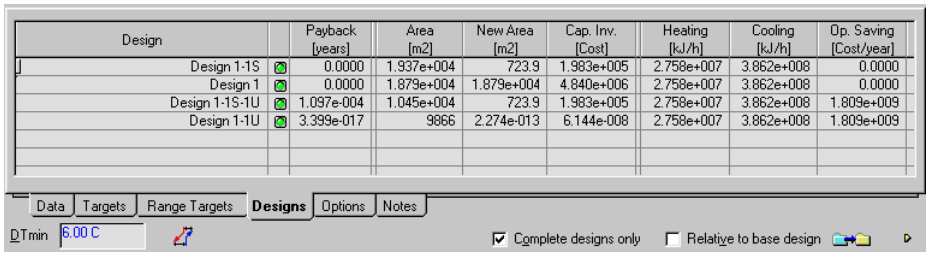
To compare retrofit design(s) with the base case, use the following procedure:



Viewer pane

1. Select the retrofit scenario in the Viewer pane.
2. Go to the **Designs** tab. The **Designs** tab contains a summary of the variables affected by the retrofit option(s).
   The Viewer pane contains the base case and three complete retrofitted designs.

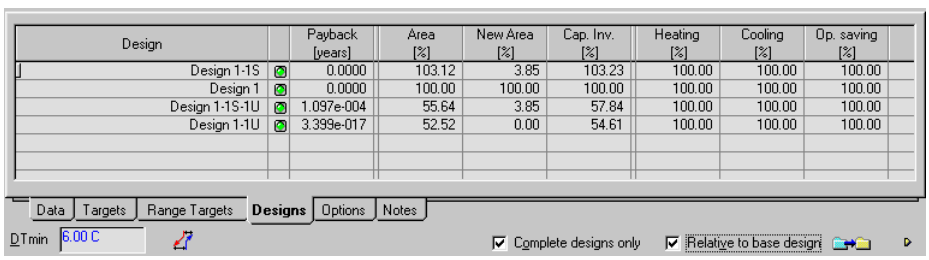
Figure 8.28



Design	Payback [years]	Area [m2]	New Area [m2]	Cap. Inv. [Cost]	Heating [kJ/h]	Cooling [kJ/h]	Op. Saving [Cost/year]
Design 1-1S	0.0000	1.937e+004	723.9	1.983e+005	2.758e+007	3.862e+008	0.0000
Design 1	0.0000	1.879e+004	1.879e+004	4.840e+006	2.758e+007	3.862e+008	0.0000
Design 1-1S-1U	1.097e-004	1.045e+004	723.9	1.983e+005	2.758e+007	3.862e+008	1.809e+009
Design 1-1U	3.399e-017	9866	2.274e-013	6.144e-008	2.758e+007	3.862e+008	1.809e+009

3. Do one of the following:
   - Check the **Complete designs only** checkbox to compare only the completed/feasible designs in the retrofit scenario.
   - Uncheck the **Complete designs only** checkbox to compare all the designs in the retrofit scenario.
4. Check the **Relative to base design** checkbox to view the summary data in percentage terms relative to the base case.

Figure 8.29



Design	Payback [years]	Area [%]	New Area [%]	Cap. Inv. [%]	Heating [%]	Cooling [%]	Op. saving [%]
Design 1-1S	0.0000	103.12	3.85	103.23	100.00	100.00	100.00
Design 1	0.0000	100.00	100.00	100.00	100.00	100.00	100.00
Design 1-1S-1U	1.097e-004	55.64	3.85	57.84	100.00	100.00	100.00
Design 1-1U	3.399e-017	52.52	0.00	54.61	100.00	100.00	100.00

The following table lists and describes the different variables available in the Designs tab for retrofit mode:

Column	Description
Payback	Displays the number of years that it will take to recover the capital cost investment.
Area	Displays the total heat transfer area of all heat exchangers in the design.
New Area	Displays the new heat transfer area that is added on the area available from existing exchangers due to the retrofit option(s).
Cap. Inv.	Displays the capital investment required for the design. This is the cost of adding new heat exchanger area, based on the economic parameters on the Economics page of the *Data* tab.
Heating	Displays the total load on hot utilities in design.
Cooling	Displays the total load on cold utilities in design.
Op. Saving	Displays the operational savings that would result from the design, as compared to the base design.

Applying Constraints

You can apply heat transfer area constraints to certain heat exchangers in the heat exchanger network (HEN), so that the retrofit options will not change the exchangers to an inapplicable/unsuitable size for the existing simulation plant.

To set the heat transfer area constraints:

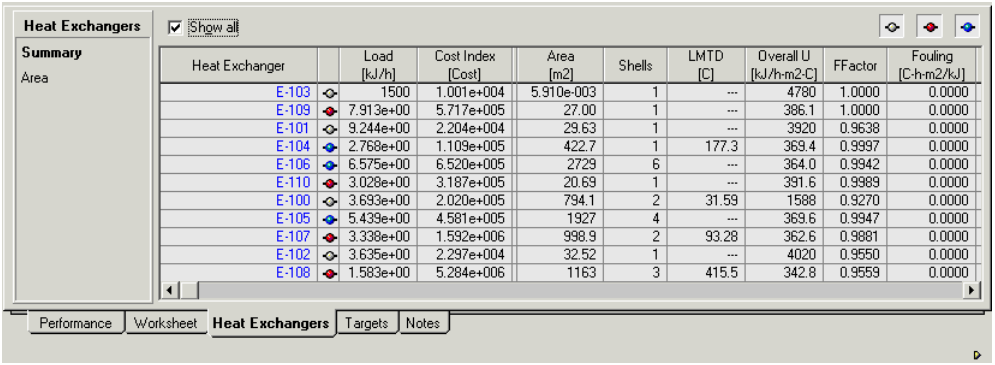
1. Enter the retrofit mode and select the base case design.
2. Click the **Heat Exchangers** tab and select the **Area** page.
3. In the appropriate cell enter the maximum spare area(s) and/or maximum added area(s) allowed for the heat exchanger(s).
4. In the **Locked** column, check the checkbox associated with the heat exchanger(s) with the limitations.
5. Apply the retrofit options to the base case design, and modifications made by the Automatic Retrofit feature will abide to the specified limitations.

Refer the **Area Page–Base Case Design** and **Area Page–Retrofitted Designs** sections for more information on where to enter the appropriate information.

Example

Consider a complete heat exchanger network (HEN)design, called Base Case, with the following list of heat exchangers:

Figure 8.30

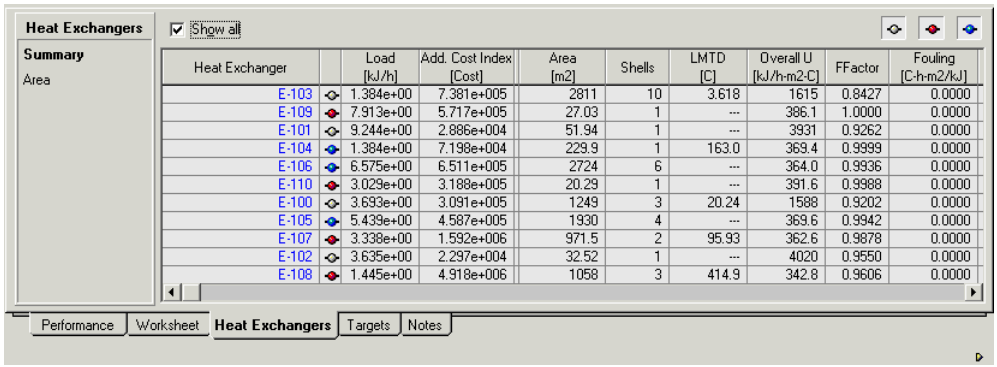


Heat Exchanger	Load [kJ/h]	Cost Index [Cost]	Area [m2]	Shells	LMTD [C]	Overall U [kJ/h-m2-C]	FFactor	Fouling [C-h-m2/kJ]
E-103	1500	1.001e+004	5.910e-003	1	---	4780	1.0000	0.0000
E-109	7.913e+00	5.717e+005	27.00	1	---	386.1	1.0000	0.0000
E-101	9.244e+00	2.204e+004	29.63	1	---	3920	0.9638	0.0000
E-104	2.768e+00	1.109e+005	422.7	1	177.3	369.4	0.9997	0.0000
E-106	6.575e+00	6.520e+005	2729	6	---	364.0	0.9942	0.0000
E-110	3.028e+00	3.187e+005	20.69	1	---	391.6	0.9989	0.0000
E-100	3.693e+00	2.020e+005	794.1	2	31.59	1588	0.9270	0.0000
E-105	5.439e+00	4.581e+005	1927	4	---	369.6	0.9947	0.0000
E-107	3.338e+00	1.592e+006	998.9	2	93.28	362.6	0.9881	0.0000
E-102	3.635e+00	2.297e+004	32.52	1	---	4020	0.9550	0.0000
E-108	1.583e+00	5.284e+006	1163	3	415.5	342.8	0.9559	0.0000

Enter the retrofit mode with HEN design as the base case and apply the Repiping retrofit option.

A retrofit design named Base Case-1P is generated along with new area values for the heat exchangers.

Figure 8.31

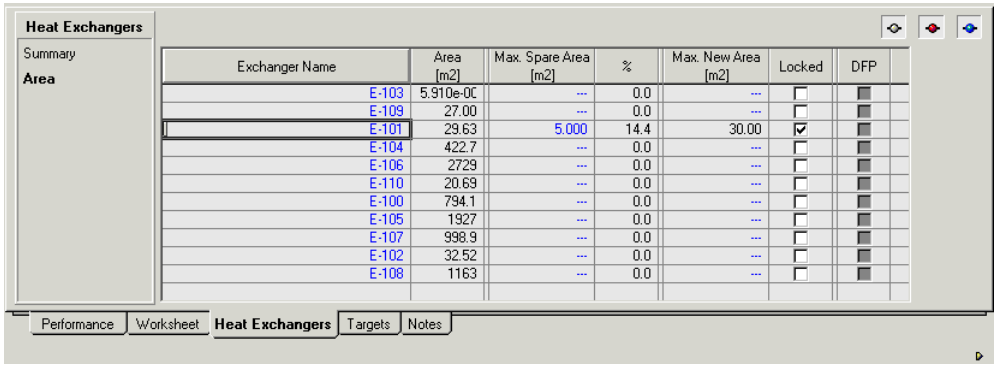


Heat Exchanger	Load [kJ/h]	Add. Cost Index [Cost]	Area [m2]	Shells	LMTD [C]	Overall U [kJ/h-m2-C]	FFactor	Fouling [C-h-m2/kJ]
E-103	1.384e+00	7.381e+005	2811	10	3.618	1615	0.8427	0.0000
E-109	7.913e+00	5.717e+005	27.03	1	---	386.1	1.0000	0.0000
E-101	9.244e+00	2.886e+004	51.94	1	---	3931	0.9262	0.0000
E-104	1.384e+00	7.198e+004	229.9	1	163.0	369.4	0.9999	0.0000
E-106	6.575e+00	6.511e+005	2724	6	---	364.0	0.9936	0.0000
E-110	3.029e+00	3.188e+005	20.29	1	---	391.6	0.9988	0.0000
E-100	3.693e+00	3.091e+005	1249	3	20.24	1588	0.9202	0.0000
E-105	5.439e+00	4.587e+005	1930	4	---	369.6	0.9942	0.0000
E-107	3.338e+00	1.592e+006	971.5	2	95.93	362.6	0.9878	0.0000
E-102	3.635e+00	2.297e+004	32.52	1	---	4020	0.9550	0.0000
E-108	1.445e+00	4.918e+006	1058	3	414.9	342.8	0.9606	0.0000

Notice the heat transfer area of heat exchangers E-101 has increased drastically due to the retrofit option ($29m^2 \rightarrow 52m^2$).

There is a limit of 30 m^2 to the heat transfer area for E-101 due to the location of the exchanger. You need to inform the Automatic Retrofit feature about this limit. You can enter the maximum area limit for exchanger E-101 in the Area page of the Base Case as shown in the figure below:

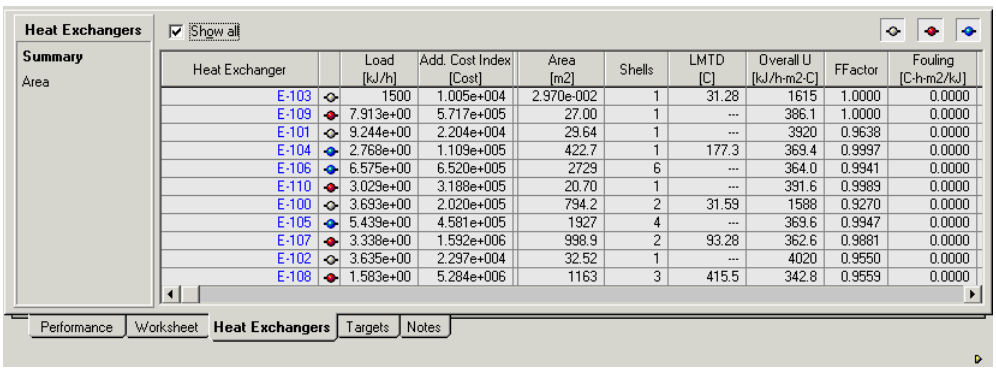
Figure 8.32



Exchanger Name	Area [m2]	Max. Spare Area [m2]	%	Max. New Area [m2]	Locked	DFP
E-103	5.910e-00	---	0.0	---	☐	
E-109	27.00	---	0.0	---	☐	
E-101	29.63	5.000	14.4	30.00	☑	
E-104	422.7	---	0.0	---	☐	
E-106	2729	---	0.0	---	☐	
E-110	20.69	---	0.0	---	☐	
E-100	794.1	---	0.0	---	☐	
E-105	1927	---	0.0	---	☐	
E-107	998.9	---	0.0	---	☐	
E-102	32.52	---	0.0	---	☐	
E-108	1163	---	0.0	---	☐	

Now when you apply the retrofit option to move both ends of exchanger to the Base Case, the Automatic Retrofit feature will take into account the specified maximum area for E-101 when generating the new retrofit design. The new retrofit design is named Base Case-2P and contains the following new area values for the heat exchangers:

Figure 8.33



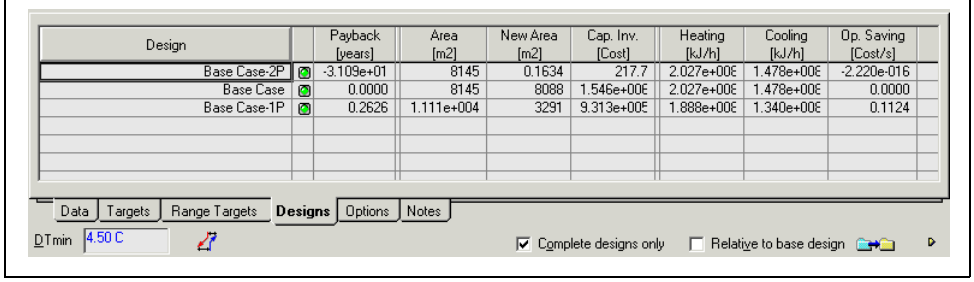
Heat Exchanger		Load [kJ/h]	Add. Cost Index [Cost]	Area [m2]	Shells	LMTD [C]	Overall U [kJ/h-m2-C]	FFactor	Fouling [C-h-m2/kJ]
E-103		1500	1.005e+004	2.970e-002	1	31.28	1615	1.0000	0.0000
E-109		7.913e+00	5.717e+005	27.00	1	---	386.1	1.0000	0.0000
E-101		9.244e+00	2.204e+004	29.64	1	---	3920	0.9638	0.0000
E-104		2.768e+00	1.109e+005	422.7	1	177.3	369.4	0.9997	0.0000
E-106		6.575e+00	6.520e+005	2729	6	---	364.0	0.9941	0.0000
E-110		3.029e+00	3.188e+005	20.70	1	---	391.6	0.9989	0.0000
E-100		3.693e+00	2.020e+005	794.2	2	31.59	1588	0.9270	0.0000
E-105		5.439e+00	4.581e+005	1927	4	---	369.6	0.9947	0.0000
E-107		3.338e+00	1.592e+006	998.9	2	93.28	362.6	0.9881	0.0000
E-102		3.635e+00	2.297e+004	32.52	1	---	4020	0.9550	0.0000
E-108		1.583e+00	5.284e+006	1163	3	415.5	342.8	0.9559	0.0000

The heat transfer area of E-101 has now been limited to the maximum value set in the Area page.

Applying limits to the heat transfer area of E-101 has caused other exchangers' areas to increase drastically as compensation (e.g., Furnace and E-104).

Next you can compare the two retrofitted designs with the base case and see how applying the constraint affects the repiping of the exchanger.

Figure 8.34



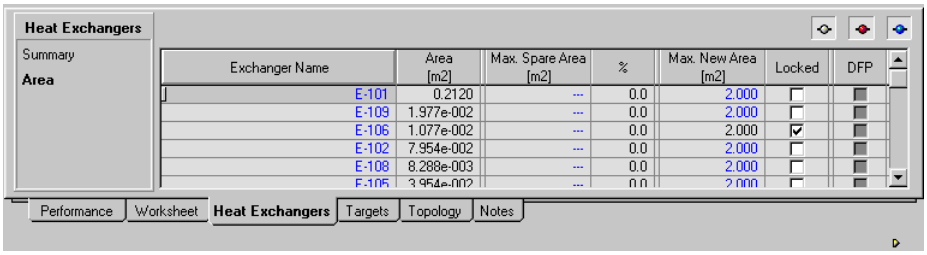
When you applied the limit on the heat transfer area, you forced the Automatic Retrofit feature to find an alternate repiping sequence that helps you reduce the total heat transfer area required and requires zero years to payback the capital investment.

The next two sections describe in detail all the objects and options available in the Area page for both the base case and retrofitted designs.

Area Page—Base Case Design

The Area page on the Heat Exchangers tab allows you to specify additional information about the area for all heat exchangers.

Figure 8.35



Unless it is custom-built, exchangers come in pre-defined sizes, which could be larger than the area required. The Area page allows you to specify the extra area in the exchanger, as well as the maximum new area you want to add to that exchanger.

The following table lists and describes the objects available in the Area page:

Object	Description
Exchanger Name column	Displays the name of the heat exchanger, as defined on the Worksheet tab or in the Heat Exchanger property view.
Area column	Displays the area of the heat exchanger as calculated or defined in the Grid Diagram.
Max. Spare Area column	Displays the maximum spare area for the associated heat exchanger.
% column	Displays the calculated spare area as a percentage of the total area.
Max New Area column	Displays the maximum new area that can be added to this heat exchanger during retrofit. The value may be required due to space limitations in the plant.
Locked column	Contains a checkbox that allows you to lock or free the heat exchanger area. HX-Net will not attempt to modify area of exchangers that are locked.
DFP column	Contains a grey box icon ■ that opens the driving force plot for the associated heat exchanger when clicked.

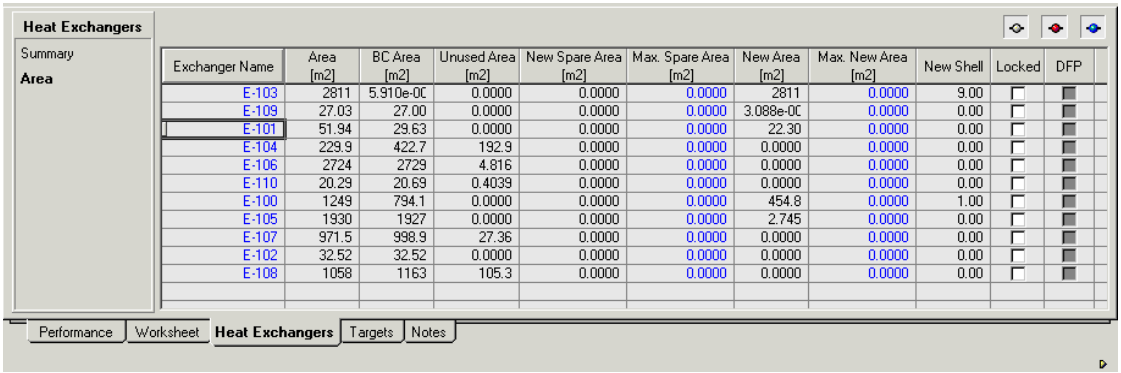
The maximum spare area may be required because manufacturers build heat exchangers at pre-defined sizes. Plants therefore have to buy heat exchangers that are larger than actually required.

For example, if you have a heat exchanger that must have a fixed area (a reboiler in a distillation column), you can lock the area.

Area Page—Retrofitted Designs

For a retrofitted design, the Area page on the Heat Exchangers tab displays all important information regarding the area of each individual heat exchanger.

Figure 8.36



Exchanger Name	Area [m2]	BC Area [m2]	Unused Area [m2]	New Spare Area [m2]	Max. Spare Area [m2]	New Area [m2]	Max. New Area [m2]	New Shell	Locked	DFP
E-103	2811	5.910e-0(	0.0000	0.0000	0.0000	2811	0.0000	9.00		
E-109	27.03	27.00	0.0000	0.0000	0.0000	3.088e-0(	0.0000	0.00		
E-101	51.94	29.63	0.0000	0.0000	0.0000	22.30	0.0000	0.00		
E-104	229.9	422.7	192.9	0.0000	0.0000	0.0000	0.0000	0.00		
E-106	2724	2729	4.816	0.0000	0.0000	0.0000	0.0000	0.00		
E-110	20.29	20.69	0.4039	0.0000	0.0000	0.0000	0.0000	0.00		
E-100	1249	794.1	0.0000	0.0000	0.0000	454.8	0.0000	1.00		
E-105	1930	1927	0.0000	0.0000	0.0000	2.745	0.0000	0.00		
E-107	971.5	998.9	27.36	0.0000	0.0000	0.0000	0.0000	0.00		
E-102	32.52	32.52	0.0000	0.0000	0.0000	0.0000	0.0000	0.00		
E-108	1058	1163	105.3	0.0000	0.0000	0.0000	0.0000	0.00		

The following table lists and describes the objects available in the Area page:

Object	Description
Exchanger Name column	Displays the name of the heat exchanger, as defined on the Worksheet tab or in the Heat Exchanger property view.
Area column	Displays the area of the heat exchanger as calculated or defined in the Grid Diagram.
BC Area column	Displays the area of the same heat exchanger in the base case design.
Unused Area column	Displays unused area of the heat exchanger if the new heat exchanger area is less than the base case exchanger area.
New Spare Area column	Displays the total spare area obtained after implementing new HEN design.
Max Spare Area column	Displays the maximum spare area for the heat exchanger.
New Area column	Displays the new area required if the heat exchanger in the design is larger than the exchanger in the base case.
Max New Area column	Displays the maximum new area that can be added to this heat exchanger during retrofit. The value may be required due to space limitations in the plant.
New Shell column	Displays the number of new shells required if the heat exchanger in the current design is larger than the one in the base case.

The maximum spare area is required because manufacturers build heat exchangers at pre-defined sizes. Plants therefore have to buy heat exchangers that are larger than actually required.

For example, if you have a heat exchanger that must have a fixed area (a reboiler in a distillation column), you can lock the area.

Object	Description
Locked column	Contains a checkbox that allows you to lock or free the heat exchanger area. HX-Net will not attempt to modify area of exchangers that are locked.
DFP column	Contains a grey box icon that opens the driving force plot for the associated heat exchanger when clicked.

9 Size & Cost Assumptions

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9.1 Introduction

The program's costing methods provide relative costs of the design options and not the exact costs.

For more detailed costing, the program recommends the HYSYS Economix software package.

The program allows you to determine the size and cost of columns and heat exchangers. The methods used in the size and cost calculations are developed for the preliminary configuration analysis (i.e., the focus is on the relative comparison of various design options, and not the absolute costs).

The program's sizing methods use the following approximations:

- The column vapour flow rates are calculated for each section, not for each tray.
- The diameter is predicted using a simple correlation of flooding velocity and the physical properties for each section, not by performing rigorous calculations based on each tray.
- The condensers and reboilers are approximated using single shell heat exchanger sizing and costing models. These models do not account for the type of reboiler or condenser and assume a single pass heat exchanger.

The costing methods are semi-empirical and simplified. The typical accuracy of the costing estimates is $\pm 30\%$.

The sizing and costing options are contained in two views: Capital Cost and Utility Database.

For more information, refer to **Section 10.1 - Capital Cost View** and **Section 10.2 - Utility Database View** from the **User Guide**.

The sizing and costing feature is limited to the following operations:

- Azeotropic Column Sequencing
- Column Sequencing
- Simple Column
- Three Product System
- Complex Column

The cost option is divided into two sections:

- **Capital cost**. This cost is also called fixed cost or capital expenditure (CapEx), and is a one-time investment. For example, the cost of purchasing and installing equipment would be considered a capital cost.
- **Operation cost**. This cost is also called variable cost or operating expenditure (OpEx), and is time dependant. For example, the cost of energy used to operate equipment would be considered an operation cost.

9.2 Capital Cost of a Column

The capital cost associated with the column (i.e., column shell, trays, platform and ladders) is estimated using costing correlations (cost as a function of weight, diameter and height of the column shell) provided by Mulet et al (1981b)[102].

In calculating the capital cost of a column, the program considers the following costs:

- Cost of the vessel of the column
- Cost of all the trays in the column
- Cost of the ladder and platform
- Cost of installing the column

The first step in the capital cost estimation is to size the equipment to identify critical dimensions such as the height and the diameter of the column shells, etc. These dimensions are used with a number of design specifications to predict size details for the equipment, such as column shell thickness and the weight of the shell required for the design, etc. The capital investment required to purchase basic equipment is then estimated using empirical and historical cost correlation. The purchase cost is then multiplied with an appropriate installation factor to cover the cost of auxiliary items such as instrumentation, piping, and nozzles, and supplementary costs, such as foundation, insulation, and lighting.

For more information about the Capital Cost view, refer to **Section 10.1 - Capital Cost View** from the **User Guide**.

All information related to sizing and costing is available in the Capital Cost view. The program provides the default values for all sizing and costing parameters. The coefficients of the costing models are in SI units and these coefficient values do not change when you select a different system of units in the Session Preferences view.

For more information about the Session Preferences view, refer to **Section 5.4 - Preferences** from **User Guide**.

If you change the units in the Session Preferences view, you may have to manually change some coefficient values in the Capital Cost view.

The following table lists the Capital Cost view coefficients that may require manual adjustment if you change the units:

The table also includes the location of the coefficients in the Capital Cost view, and the equations that the coefficients correspond to.

Refer to **Section 10.1.2 - Column Tab** from the **User Guide** for more information.

Tab	Page	Coefficients	Equation
Column	**Vessel Cost**	Coeff A Coeff B Coeff C Coeff D	**Equation (9.10)**
	Tray Cost	Coeff A Coeff B Coeff C Coeff D	**Equations (9.12)** and **(9.13)**
	Misc. Cost	Coeff A Coeff B Coeff C	**Equation (9.14)**
	Installation	Lower Limit for Purchase Cost Upper Limit for Purchase Cost Coeff A Coeff B Coeff C Coeff D Coeff E	**Equation (9.15)**

The following sections explain in more detail the calculation of the column dimension, vessel cost, tray cost, miscellaneous cost, and installation factor.

9.2.1 Column Sizing

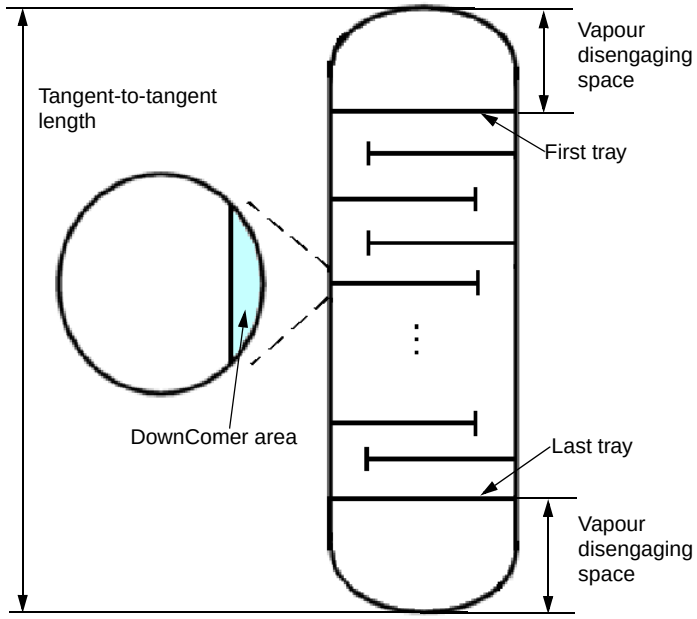
The performance models of the column (e.g., Fenske-Underwood method) provide information (e.g., number of trays and reflux requirements) needed to achieve the desired separation. This information is used to calculate preliminary column sizing information.

This sizing model uses the following design parameters:

- **Tray type**. The program accommodates several tray types (valve, bubble cap, and sieve) by allowing you to manipulate the tray costing coefficient values.
- **Tray spacing**. The flooding velocity and the column height depend on the tray spacing. Higher tray spacing allows higher flooding velocity but requires a taller column.

- **Tray layout**. Geometrical information about the tray, like downcomer area fraction and fractional hole area, is used to predict the flooding velocity and column diameter. See the figure below.

Figure 9.1

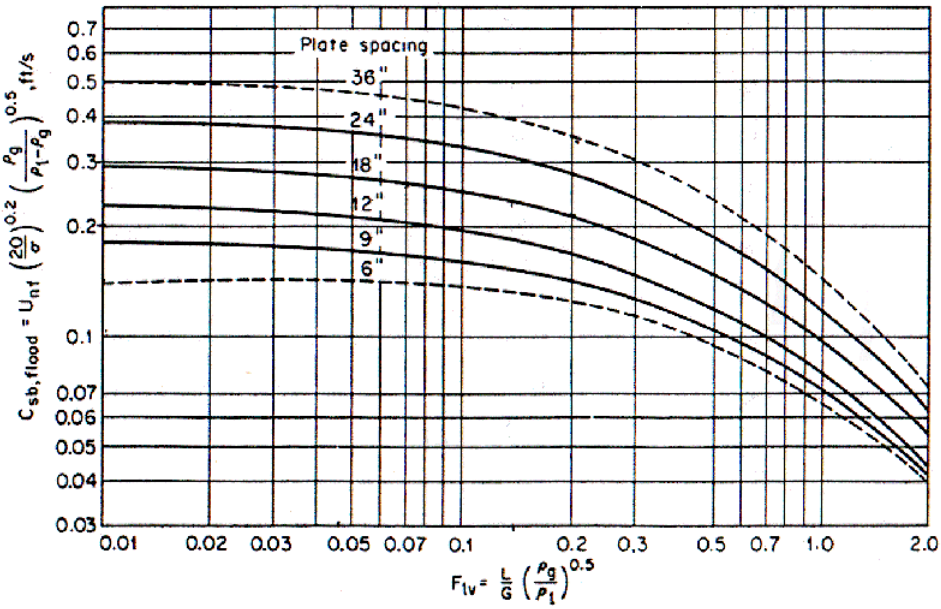


- **Physical properties**. This includes molar and mass densities, surface tension, etc., of the vapour and liquid streams.
- **Vapour disengaging space**. This is the space above the top tray and below the bottom tray. This space minimizes the entrainment losses at the top and bottom section of the column. It is used when determining the column height.
- **Flooding factor**. This refers to the operating vapour velocity as a fraction of flooding velocity. A higher value for the flooding factor will decrease the column diameter but increase the possibility of column flooding.
- **Tray efficiency**. This relates the number of theoretical stages to the actual number of stages in the column.

These parameters plus the vapour flow are used to predict the flooding velocity of the system. The program employs a simplified correlation that relates the flow parameter (defined as the X-axis on a plot) and tray layout with the flooding velocity.

The following figure shows the plot of flooding velocities for different tray spacing when valve trays are used.

Figure 9.2



J.R. Fair, Petro/Chem Eng. 33 (10), p. 45, 1961, Petroleum Engineer International, Dallas,

The design vapour velocity and the vapour load are then used to predict the column cross-sectional area.

The following equation is used to determine the column diameter:

$$D_i = \sqrt{\frac{4V_f}{\pi\nu} \times \frac{1}{(1 - A_{DC})}} \qquad (9.1)$$

where: D_i = *inside diameter of the column*

V_f = *volumetric vapour flow rate*

ν = *design vapour velocity*

A_{DC} = *downcomer area fraction*

The following equation is used to determine column height:

$$H = (N_t \times \text{tray spacing}) + (2S_v) \quad (9.2)$$

where: H = *column height*

N_t = *total number of trays in the column*

S_v = *height of the vapour disengaging space*

9.2.2 Vessel Design

The column shell is designed (i.e., the wall thickness and weight is calculated) using the procedure described by Mulet et al (1981a)[101].

When designing a column, you determine the wall thickness of the vessel/column based on wind load, corrosion allowance, vessel orientation, and whether the column has an internal pressure or no pressure (vacuum).

The following sections describe in more detail the calculations and assumptions for the variables used to calculate the actual wall thickness for the column.

Vertical Vessel

The following equation is used to determine the wall thickness of a vertical vessel column:

$$th_s = \frac{1}{2}(th_p + th_b) \times th_c \quad (9.3)$$

where: th_s = *wall thickness of the column*

th_p = *wall thickness to withstand design pressure*

th_b = *wall thickness for the bottom portion of the column*

The corrosion is assumed to occur inside the column only.

th_c = *wall thickness to allow for corrosion*

Internal Pressure

You can change the safety margin percentage in the Capital Cost view. Refer to **Section 10.1.2 - Column Tab** from the **User Guide** for more information.

If the column contains a positive pressure (pressure > 1 bar), then the wall thickness of the column is designed to withstand stress on the longitudinal seam. When you supply the pressure for the column, the program automatically increase the given pressure value by 20% (a specified pressure safety margin).

The following equation is used to determine the wall thickness at the specified pressure:

$$th_p = \frac{P_g \times R_i}{(S_{max} \times E_j) - (0.6P_g)} \tag{9.4}$$

where: P_g = *gage pressure based on the safety margin*

R_i = *inside radius of the vessel*

S_{max} = *maximum allowable stress*

E_j = *joint efficiency which takes into account the deficiencies of the welding joints.*

The maximum allowable stress represents the maximum stress force that the selected construction material can withstand before buckling/ breaking (Perry 7th ed.[108]).

You can specify different values for the maximum allowable stress and joint efficiency, or you can use the default values provided by the program. The default values from the program are based on carbon steel at a temperature range of 20° C-80° C.

Vacuum Vessel

If the column is a vacuum vessel (i.e., pressure < 1 bar), then the program assumes a fixed wall thickness.

Equation (9.6) applies to variables in SI units only.

The following equations are used to determine the wall thickness:

$$th_p = th_e + F_e \tag{9.5}$$

$$F_e = \frac{L_t \times (7.1095 D_i - 2.167)}{100000} - 4.826 \times 10^{-3} \tag{9.6}$$

where: th_e = *assumed wall thickness to withstand external pressure*

F_e = *correction factor for the wall thickness to withstand external pressure*

D_i = *inside diameter of the column*

L_t = *tangent-to-tangent length of the column*

The tangent-to-tangent length is based on the total length of the column including the sections that curve to form the cap of the column. Refer to **Figure 9.1**.

Wind Load

The wall thickness of the top portion of the column is usually thinner than the wall thickness at the bottom of the column. This is because the top of the column only has to withstand the internal or external pressure, while the wall thickness at the bottom portion of the column must withstand the wind load plus the internal or external pressure.

The following assumptions are made when calculating the additional thickness due to wind load:

- The wind load intensity is equally applied along the entire length of the column.
- The column is cylindrical, therefore the drag coefficient due to the wind resistance is 1.0.

The following equations are used to calculate the wall thickness of the bottom portion of the column:

$$th_b = th_w + th_g \tag{9.7}$$

$$th_w = \frac{\rho_a \times V_w^2 \times (D_o + F_{cl}) \times L_t^2}{S_{max} \times \pi \times D_o^2} \tag{9.8}$$

$$th_g = \frac{P_g \times R_i}{(2S_{max} \times E_j) + 0.4P_g} \tag{9.9}$$

where: th_b = *wall thickness for the bottom portion of the column*

th_w = *wall thickness required to withstand the wind load*

th_g = *wall thickness required to withstand the internal pressure at the girth seam.*

ρ_a = *density of the external medium surrounding the column*

V_w = *wind velocity*

D_o = *outside diameter of the column*

F_{cl} = *allowance factor for cage ladders attached to the column*

L_t = *tangent-to-tangent length of the column (refer to* ***Figure 9.1****)*

S_{max} = *maximum allowable stress*
This represents the maximum stress force that the selected construction material can withstand before buckling/breaking (Perry 7th ed.[108]*).*

E_j = *joint efficiency which takes into account the deficiencies of the welding joints*

P_g = *gage pressure based on the safety margin*

R_i = *inside radius of the vessel*

You can specify different values for the maximum allowable stress and joint efficiency, or use the default values provided by the program. The default values from the program are based on carbon steel at a temperature range of 20°C-80°C.

Corrosion Allowance

The corrosion is assumed to occur inside the column only.

An additional thickness value is added to the vessel's wall thickness to account for the effect of corrosion. You can manually enter the wall thickness that will be corroded or use the default value provided by the program. Refer to **Section 10.1 - Capital Cost View** from the **User Guide** for more information.

9.2.3 Vessel Cost

The program uses the diameter, height, and column shell thickness to calculate the shell volume and weight.

The cost of the vessel is correlated to the weight of the vessel. When all the dimension values for the column and the construction material density of the column are known, the program can calculate the weight and then predict the cost of the column.

The equation applies only to columns with:

- weight range of 4,090-1,060,000 kg
- inside diameter between 0.91-7.32 m
- tangent-to-tangent length between 17.53-51.82 m

The following equation is used to calculate the vessel capital cost:

$$C_s = \exp\left[A + B \times \ln(w_{ave}) + C \times \ln(w_{ave})^2 + D \times \left(\frac{L_t \times th_b}{D_i \times th_p}\right)\right] \quad (9.10)$$

where: C_s = *cost of the vessel or shell*

A, B, C = *coefficient values based on the type of material used to construct the vessel*
The default values supplied by the program for the coefficients are based on carbon steel as the construction material (Mulet, 1981[102]).

D = *coefficient value that accounts for additional cost due to different wall thickness between the top and bottom of the vessel*

w_{ave} = *average weight between the upper and lower limit weight of the vessel*
The upper and lower limit weight are determined based on the vessel's dimension multiplied with the upper and lower density of the selected construction material.

The tangent-to-tangent length is based on the total length of the column including the sections that curves to form the cap of the column. Refer to **Figure 9.1**.

D_i = *inside diameter of the column*

L_t = *tangent-to-tangent length of the column*

th_b = *wall thickness for the bottom portion of the column*

th_p = *wall thickness to withstand design pressure*

The equation used to calculate vessel capital cost also includes the cost of skirt, nozzles, and manholes.

9.2.4 Tray Cost

The program calculates the total cost of the tray based on the tray diameter, number, and construction material.

This equation set applies only to trays with diameters between 0.6-4.8 m.

The following equations are used to calculate the total tray cost:

$$C_{tt} = C_{pert} \times F_{nt} \times N_t \tag{9.11}$$

$$C_{pert} = A \times \exp(B \times D_t) \tag{9.12}$$

$$F_{nt} = \frac{C}{D \times N_t} \tag{9.13}$$

where: C_{tt} = *total tray cost*

C_{pert} = *cost per tray*

N_t = *total number of trays in the column*

F_{nt} = *number of trays factor*

D_t = *tray diameter*

A, B, C, D = coefficient values based on the type of material used to construct the tray

The number of trays factor represents the economy of scale; i.e., it takes into account that the cost of each tray decreases when you purchase more trays.

The default coefficient values supplied by the program assume carbon steel as the construction material (Mulet, 1981[102])

9.2.5 Miscellaneous Cost

The miscellaneous cost contains the cost of the ladder and platform. The cost of the ladder and platform is based on the column's diameter and the column's tangent-to-tangent length (refer to **Figure 9.1**).

The following equation is used to calculate the miscellaneous cost:

The equation applies only to a column with:

- inside diameter between 0.91-7.32 m
- tangent-to-tangent length between 17.53-51.82 m

The default coefficient values supplied by the program assume carbon steel as the construction material (Mulet, 1981[102])

$$C_{pl} = A \times (D_{ave})^{B} \times (L_{ave})^{C} \tag{9.14}$$

where: C_{pl} = *cost of the ladder and platform for the column*

A, B, C = *coefficient values based on the type of material used to construct the ladder and platform*

D_{ave} = *average diameter between the specified upper and lower limit value*

L_{ave} = *average tangent-to-tangent length between the specified upper and lower limit value*

9.2.6 Installation Factor

The installation factor includes the cost of foundation, structural, instrumentation, point, insulation, electrical and average piping.

The program calculates the installation cost by multiplying the column purchase cost with the installation factor. The installation factor in the program is a non-linear function of the column purchase cost. One of the assumptions made in calculating the installation factor is the installation factor decreases as the column purchase cost increases.

This equation set is valid for heat exchanger purchase costs between $54,000-$1,810,000 US dollars.

The following equations are used to calculate the installation factor:

$$I_{fc} = A - B \times C_f + C \times C_f^2 + \frac{D}{C_f} + \frac{E}{C_f^2} \tag{9.15}$$

$$C_f = \frac{C_{pc}}{10^6} \qquad C_{pc} = C_s + C_{tt} + C_{pl} \tag{9.16}$$

where: I_{fc} = *installation factor for column*

A = *ideal installation factor*

B, C, D, E = *coefficient values used to manipulate the installation factor so the value relates to the column purchase cost*

C_{pc} = *column purchase cost*

C_s = *cost of the vessel or shell*

C_{tt} = *total tray cost*

C_{pl} = *cost of the ladder and platform for the column*

9.3 Capital Cost of a Heat Exchanger

The capital cost for the condensers and reboilers is determined using correlations that describe cost as a function of the heat transfer area of the heat exchanger and the operating pressure. (provided by Corripio et al 1982[28]).

The first step in estimating the capital cost for heat exchangers is to calculate the size of the heat exchangers to determine the heat transfer area. The heat transfer area is used with a number of design specifications to calculate the purchase cost of the heat exchangers. The purchase cost is estimated using both empirical and historical costs. An installation factor is multiplied with the purchase cost to account for the cost of auxiliary items such as instrumentation, piping, nozzles, and supplementary costs such as foundation, insulation, and lighting.

All information related to sizing and costing is available in the Capital Cost view. The program provides the default values for all sizing and costing parameters. The coefficients of the costing models are in SI units and these coefficient values do not change when you select a different system of units in the Session Preferences view. If you change the units in the Session Preferences view, you may have to manually change some coefficient values in the Capital Cost view.

Tab	Page	Coefficients	Equation
Heat Exchanger	**Sizing**	Coeff A and Coeff B from all three tables in the Sizing page	**Equation (9.18)**
	Costing	Coeff A Coeff B Coeff C Coeff D Coeff E	**Equations (9.19)** and **(9.20)**
	Installation	Lower Limit for Purchase Cost Upper Limit for Purchase Cost Coeff A Coeff B Coeff C Coeff D Coeff E	**Equation (9.21)**

The following sections explain in more detail the calculations for the heat transfer area, design pressure cost factor, design type cost factor, heat exchanger base cost, and installation factor.

9.3.1 Heat Transfer Area

As mentioned in the previous section, the heat transfer area of the heat exchanger in the column system is a critical dimension used in calculating the capital cost of the heat exchanger.

The typical distillation column usually contains two heat exchangers: a condenser and a reboiler. The heat transfer area of the heat exchanger is calculated based on the known operating temperature, duty, heat transfer coefficient, and log mean temperature difference (LMTD) of the condenser or reboiler. The following assumptions are made regarding these calculations:

- The operating temperature and duty values for the heat exchanger are based on results previously calculated in designing the vessel and tray sections of the column.
- The heat transfer coefficient value is based on the utility selected to heat or cool the reboiler or condenser.
  You can use the set of default utilities with heat transfer coefficient values provided by the program, or you can enter your own utility and heat transfer coefficients. Refer to **Section 10.2 - Utility Database View** from the **User Guide** for more information.
- The LMTD is based on the temperature differences between the process and utility streams entering and exiting the heat exchanger.

The program will automatically select a utility for you based on the assumptions/procedure in **Section 9.4 - Operating Cost**.

The following equation is used to determine the heat transfer area for each heat exchanger in the column system:

$$A_{ht} = \frac{Q}{U \times LMTD} \tag{9.17}$$

where: A_{ht} = *heat transfer area of the heat exchanger*

Q = *total duty of the heat exchanger*

U = *heat transfer coefficient of the utility*

9.3.2 Design Pressure Factor

The effect of the operating pressure on the purchase cost is determined by multiplying the heat exchanger base cost with the design pressure cost factor.

The design pressure cost factor is a function of the operating pressure and the required heat transfer area. As the operating pressure increases, the design pressure cost factor increases.

The following equation is used to determine the design pressure cost factor:

The equation is valid for heat transfer area between 14m^2-1,100 m^2.

$$F_p = A + B \times \log A_{ht} \quad (9.18)$$

where: F_p = *design pressure cost factor*

The program provides default coefficient values for three different sets of pressure ranges. The program will automatically select the appropriate coefficient values based on the heat exchanger operating pressure.

A, B = *coefficient values used to calculate the* F_p
The coefficient values are dependent on the operating pressure. Refer to Corripio et al, 1982[28] *for more information.*

A_{ht} = *total heat transfer area required for the heat exchanger to function as specified*

9.3.3 Type of Heat Exchanger

The effect of the type of heat exchanger on the purchase cost is determined by multiplying the heat exchanger base cost with the design type cost factor.

The design type cost factor is a function of the heat exchanger type selected and the required heat transfer area. The program accommodates fixed head, kettle reboiler, and U-tube heat exchangers by allowing you to manipulate the heat exchanger costing coefficient values.

The equation is valid for heat transfer area between 14 m^2-1,100 m^2.

The following equation is used to determine the design type cost factor:

$$F_{dt} = \exp[D + E \times \log A_{ht}] \quad (9.19)$$

where: F_{dt} = *design type cost factor*

The program provides default coefficient values for a fixed head heat exchanger.

D, E = *coefficient values used to calculate* F_{dt}
The coefficient values are dependent on the type of heat exchanger selected. Refer to Corripio et al, 1982[28] *for more information.*

A_{ht} = *total heat transfer area required for the heat exchanger to function as specified*

9.3.4 Base Cost of Heat Exchanger

The base cost of the heat exchanger is a function of the heat transfer area, and is used as a starting point to calculate the purchase cost of the heat exchanger. The purchase cost of the heat exchanger is determined by multiplying the base cost with the design pressure cost factor and the design type cost factor.

The base cost of the heat exchanger includes the cost of a floating-head shell-and-tube exchanger, ladder, and platform.

The equation is valid for heat transfer area between 14 m^2-1,100 m^2.

The following equation is used to calculate the base cost:

$$C_b = \exp[A + B \times \log A_{ht} + C \times (\log A_{ht})^2] \quad (9.20)$$

where: C_b = *base cost of the heat exchanger*

The program provides the default coefficient values for the construction material of carbon steel and the assumed operating pressure at 700 kN/m^2.

A, B, C = *coefficient values used to calculate the* C_b
The coefficient values are dependant on the heat exchanger construction material (Mulet et al 1981[102]*).*

A_{ht} = *total heat transfer area required for the heat exchanger to function as specified*

9.3.5 Installation Factor

The installation factor includes the cost of foundation, structural, instrumentation, point, insulation, electrical and average piping.

The program calculates the installation cost by multiplying the heat exchanger purchase cost with the installation factor. The installation factor in the program is a non-linear function of the heat exchanger purchase cost. One of the assumptions made in calculating the installation factor is that the installation factor decreases as the heat exchanger purchase cost increases.

This equation set is valid for a heat exchanger purchase cost between $9,500-$240,000 US dollars.

The following equation is used to calculate the installation factor:

$$I_{fx} = A - B \times C_f + C \times C_f^2 + \frac{D}{C_f} + \frac{E}{C_f^2} \tag{9.21}$$

$$C_f = \frac{C_{px}}{10^6} \qquad C_{px} = C_b + F_{dt} + F_p \tag{9.22}$$

where: I_{fx} = *installation factor for heat exchangers*

A = *ideal installation factor*

B, C, D, E = *coefficient values used to manipulate the installation factor so that the value relates to the heat exchanger purchase cost*

C_{px} = *heat exchanger purchase cost*

C_b = *base cost of the heat exchanger*

F_{dt} = *design type cost factor*

F_p = *design pressure cost factor*

9.4 Operating Cost

The purpose of the operating cost module is to estimate the heating and cooling costs associated with the separation system. It allows users to define available process utilities (such as steam, cooling water, etc.) and identify the trade-offs related to quality and quantity of the energy. It assumes that all the heating and cooling requirements of the separation system are satisfied by process utilities for which the supply is unlimited.

The operating cost of the column includes the cost of supplying heat to the reboiler and the cost of removing heat from the condenser. The temperature of the condenser and/or reboiler is obtained from the previous calculations and used to identify the feasible utilities. If none of the available utilities is feasible, then the operating cost will be set to zero.

9.4.1 Required Utility Information

Refer to **Section 10.2 - Utility Database View** from the **User Guide** for information about how to enter required utility information.

The following is a list of information required for a utility to be used in the heat exchanger:

- **Name**. The utility names identify and differentiate one utility from another.
- **Inlet Temperature**. The utility requires an inlet temperature as it flows into the heat exchanger.
- **Outlet Temperature**. The utility requires an outlet temperature as it flows out of the heat exchanger. The outlet temperature is always different than the inlet temperature.

  If $T_{in} > T_{out}$ then the utility is called a Hot utility and can be used to supply heat. If $T_{in} < T_{out}$ then the utility is called a Cold utility and can be used to remove heat.

where: T_{in} = *inlet temperature*

T_{out} = *outlet temperature*

- **Delta T min**. The Delta T min is the minimum approach temperature required when the utility is used to supply or remove heat. According to thermodynamic feasibility criteria, the Delta T min value must be greater than 0°C, but for practical reasons its value should be greater than 1°C.
- **Heat Transfer Coefficient**. The heat transfer coefficient (HTC) value is the effective HTC that is used for calculating the area of the condenser or reboiler when that process utility is used.
- **Cost Index**. The cost index represents the cost of supplying (for a hot utility) or removing (for a cold utility) a unit quantity of energy. This value is used with the condenser or reboiler duty to predict the cost of running or operating the heat exchanger.

9.4.2 Calculating Applicable Limits

Application Range Low (ARL)
Application Range High (ARH)

Once the required information for each available utility is provided, the operating cost module will calculate the Applicable Limits (ARL & ARH) for each utility. The ARH & ARL temperature calculations consider the overall system to identify the feasible temperature range the process utility can serve.

- One limit is identified from the thermodynamic limitation (i.e., the approach temp must be > the specified *delta T* of the utility).
- The other limit is obtained using the Exergy principle. The low temperature hot utility is preferred when more than one hot utility is feasible. Similarly, the high temperature cold utility is preferred when more than one cold utility is feasible.

ARL & ARH are calculated using following formulas:

For heating:

$$ARH = T_{iu} - \Delta T_{min} \qquad (9.23)$$

$$ARL \leq \text{exiting temperature} \leq ARH$$

For cooling:

$$ARL = T_{ou} + \Delta T_{min} \qquad (9.24)$$

$$ARH \geq \text{exiting temperature} \geq ARL$$

where: T_{iu} = *inlet temperature of the utility*

ΔT_{min} = *minimum temperature difference*

T_{ou} = *outlet temperature of the utility*

The following sample calculation of the ARH & ARL demonstrates the results of the previous formulas.

Assume that a process site has the following hot utilities:

Hot Utility	T_{iu} (°C)	T_{ou} (°C)	ΔT_{min}
LP steam	125	124	10
MP steam	175	174	15
HP steam	250	249	20

- To heat a stream to 115°C, you can select LP steam, MP steam, or HP steam. Based on the Exergy principle, LP steam will be preferred. Example calculation for LP steam: $ARH = T_{iu} - \Delta T_{min} = 115$ and $ARL = -273$.
- To heat a stream with a temperature above 115°C but below 160°C, you can select MP steam or HP steam. Based on the Exergy principle, MP steam will be preferred. Example calculation for MP steam: $ARH = T_{iu} - \Delta T_{min} = 160$ and $ARL = 115$.
- To heat a stream with a temperature above 160°C but below 230°C, you can use only HP steam. Example calculation for HP steam: $ARH = T_{iu} - \Delta T_{min} = 230$ and $ARL = 160$.
- This process site does not contain any suitable process utility to heat a stream where the temperature is above 230°C.

9.4.3 Selecting a Utility (by-default)

To access/manipulate the information in the default utility database in the program, refer to **Section 10.2 - Utility Database View** from the **User Guide**.

The program supplies a set of default utilities in a utility database file (utildatabase.hud). The costing and characteristic information of the default utilities are also included in this utility database file.

The program uses the following procedure to select the utility type for the condenser or reboiler:

1. The program uses the temperature of the condenser or reboiler to identify a list of feasible cold or hot utilities.
2. Out of the list of feasible utilities, the program selects the utility with the lowest cost index.

As the final utility type selection is based solely on the lowest operating cost, the utility type selected might require a large heat transfer area. This could increase the heat exchanger capital cost and require more space than what you had allocated for the heat exchanger unit.

You can select a different utility type by entering the Simple Column or Complex Column views. Refer to **Section 1.1.5 - Utility Selection for Condenser/ Reboiler** of the Separation manual for more information.

If you change the utility type and reduce the heat exchanger size, this could decrease capital cost but may increase the operating cost.

9.4.4 Default Utility Database

The default utility database in the program contains utilities typically available on the process site. The utilities in the utility database accommodate the entire range of heating and cooling temperatures.

The default cost indices of the hot and cold utilities are obtained by following simplified calculations presented in Douglas, 1980[37], and the natural gas price in North America 1990.

The calculation assumes that the steam is always generated from the boiler feed water (BFW) and does not account for the complexities related to turbines or heat and power trade-offs.

The program assumes an average film value between the reported film coefficient on the utility side and the overall film coefficient.

The default values for the heat transfer coefficients (HTC) in the utility database are taken from Table 3.3 - Film coefficient used for shell-and-tube heat exchangers on page 146 of the User Guide on Process Integration for the Efficient Use of Energy, Institution of Chemical Engineers. Rugby, UK (1994).

Each operating site has it's own unique utility network, so the costs of the utility will be different for each site. For example, if a site has a steam turbine that produces LP steam in its exhaust, then the LP steam will be very cheap compared to the site that generates LP steam from BFW. The program recommends that you should define all utility data (cost, temperatures, etc.) based on your operating site and save that data as a utility database (*.hud) file. This file can be easily recalled and reused for different cases. Refer to **Section 10.2 - Utility Database View** from the **User Guide** for more information.

9.4.5 Shaft Work Model

The shaft work value is calculated using the Carnot cycle. The Carnot cycle consist of four steps: two isothermal and two adiabatic. The steps are:

1. Isothermal step occurs at the heat sink (heat being absorbed by the work fluid).
2. Adiabatic step occurs in a form of work (heat absorbed in the work fluid is used to produce work force).
3. Isothermal step occurs at the heat source (heat in the work fluid is removed).
4. Adiabatic step occurs in a form of work (work force is applied to the the work fluid).

The following equation is used to calculate the work force:

$$W = \left(1 - \frac{T_c}{T_h}\right) Q_h \tag{9.25}$$

where: W = *work force (shaft work)*

T_c = *temperature of the cold stream*

T_h = *temperature of the hot stream*

Q_h = *heat load that needs to be absorbed by the work fluid*

9.5 Economic Factors

For more information on the TAC, refer to Douglas 1980[37].

After the purchase and installation costs for the column have been determined, the program calculates the total annual cost (TAC) of the column. The TAC is a sum of the annualized capital cost and tax rebated operating cost, and it takes into account the following:

- **Interest rate**. This is the time value of money.
- **Plant life**. This is the operational life of the plant or time period for which the plant operates.
- **Inflation**. This is the change of equipment value over time.
- **Total cost of the column**. This includes the purchase and installation costs.

The tax rebated operating cost takes into account the income tax and the utility/operating cost, and uses the following formulas:

$$TAC = F_{an} \times C_{cc} + (1 - F_{it}) \times \text{operating cost} \tag{9.26}$$

$$C_{cc} = (I_{fc} \times C_{pc}) + (I_{fx} \times C_{px})_{\text{condenser and reboiler}} \tag{9.27}$$

$$F_{an} = \frac{i_r \times (1 + i_r)^{PL}}{(1 + i_r)^{PL} - 1} \tag{9.28}$$

where: C_{cc} = *total capital cost of the column(s) and heat exchangers*

Depending on the type and number of columns there might be more than one condenser and reboiler.

I_{fc}, I_{fx} = *installation factor for column and heat exchangers*

C_{pc}, C_{px} = *column(s) and heat exchangers purchase cost*

F_{an} = *annualization factor*

i_r = *interest rate*

PL = *plant life in years*

F_{it} = *income tax factor*

The impact of inflation is accounted for using the Marshall and Swift Index, which is applied to the total cost. The program allows you to enter a base year and the current cost. The Marshall and Swift Index cost values can be found in the front or back section of the Chemical Engineer journals.

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