CHAPTER TWO
OVERALL MASS TARGETING

In many cases, it is useful to determine the potential improvement in the performance of a whole process or sections of the process without actually developing the details of the solution. In this context, the concept of targeting is very useful. Targeting is aimed at benchmarking the performance of a process ahead of detailed design and without commitment to the specific details of the strategies leading to improvement. This priori approach ensures that the process capabilities are explored without exhausting the designer’s time and effort. Examples of important mass targets include minimum consumption of material utilities (solvents, water, etc.), minimum discharge of wastes, minimum purchase of fresh raw materials, minimum production of undesirable byproducts, and maximum sales of desirable products.

To illustrate the concept of overall mass targeting, let us start by considering the objective of minimizing the discharge of a waste. Later, other objectives will be discussed.

TARGETING FOR MINIMUM DISCHARGE OF WASTE

Consider the case when it is desired to determine the target for minimizing the load of a discharged species (e.g., pollutants in effluents). Three sets of data for that species are first collected: fresh usage, generation/depletion, and terminal discharge. The fresh usage (F) corresponds to the quantity of the targeted species in streams entering the process (the waste stream may have entered the process as a fresh feedstock or a material utility). Within any process, several phenomena contribute to the net balance of a species. Generation (G) refers to the net amount of the targeted species which is produced through chemical reaction. Depletion (D) may take place through chemical reactions but it may also be attributed to leaks, fugitive emissions, and other losses that are not explicitly accounted for. The net generation (Net_G) of a targeted species is defined as the difference between generation and depletion. Therefore,

$$Net\_G = G - D \tag{2.1}$$

. Finally, the terminal discharge (T) is used to refer to the load of the targeted species in streams designated as waste streams or point sources for pollution.

An overall material balance on the targeted species before mass integration (BMI) is shown in Fig. 1 and can be expressed as:

$$T^{BMI} = F^{BMI} + Net\_G^{BMI} \tag{2.2}$$

where T^{BMI}, F^{BMI}, and Net_G^{BMI} respectively refer to the terminal load, fresh load, and net generation of the targeted species before any mass integration changes.

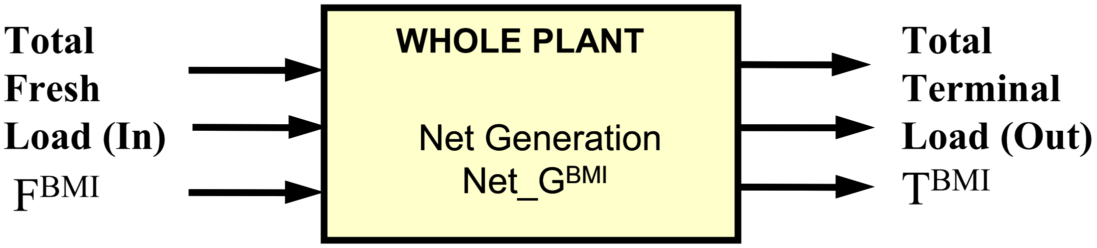

Fig. 2.1. Overall Material Balance For the Targeted Species Before Mass Integration

In order to reduce the terminal discharge of the targeted species, the two terms on the right hand side of Eq. (2.2) are to be reduced. The general solution strategy is described by Noureldin and El-Halwagi (1999). However, there are several special cases for which simplified targeting methods can be developed. For instance, when the net generation is independent of stream recycle and adjustments in fresh feed, we can use the following two-step shortcut method to identify the minimum-discharge target. In the first step, the net generation of the targeted species is minimized. The net generation can be described in terms of the process design and operating variables that are allowed to be modified. The value of the minimum net generation of the targeted species is referred to as Net_G^{MIN}. As can be seen from Fig. 2.2., once the net generation has been minimized we can calculate the terminal discharge load after generation minimization (T^{AGMIN}) through an overall material balance:

$$T^{AGMIN} = F^{BMI} + Net\_G^{MIN} \tag{2.3}$$

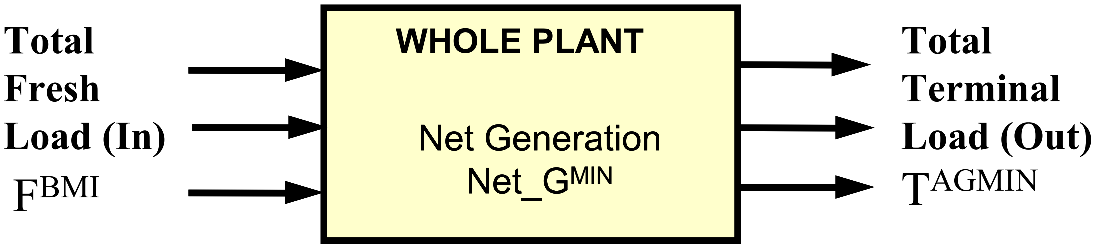

Fig. 2.2. Overall Material Balance For the Targeted Species After Minimizing the Net Generation

In the second step, the fresh usage in the process is minimized. First, the requirement for a fresh supply of the targeted species is reduced to the extent feasible by adjusting design and operating variables of the units that employ the targeted species in fresh streams. This entails answering the following questions:

- What are the design and operating variables that influence fresh usage?
- Which of these variables are allowed to be changed (manipulated variables)?
- What is the functional relationship between these variables and fresh consumption? This relationship may be expressed as:

$$F = f(\text{manipulated design variables, manipulated operating variables}) \tag{2.3a}$$

Equation (2.3a) can be minimized to identify the minimum load of the targeted species in the fresh feeds after reduction (referred to as F^{AFR}). As can be seen from Fig. 2.3., the terminal load after minimization of net generation and reduction in fresh feed is expressed as:

$$T^{AGMIN, AFR} = F^{AFR} + Net\_G^{MIN} \tag{2.3b}$$

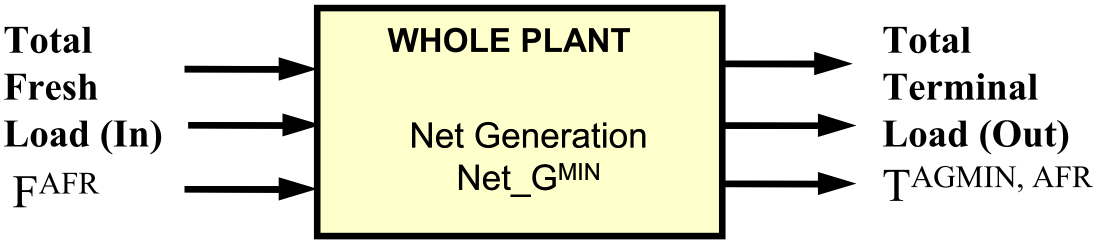

Fig. 2.3. Overall Material Balance of the Targeted Species after Fresh Reduction and Net-Generation Minimization

Finally, it is possible to recover almost all of the targeted species from the terminal streams or from paths leading to the terminal streams and render the recovered species in a condition which enables its use in lieu of the targeted species in the fresh feed. Clearly, the higher the recovery and recycle to replace the fresh load, the lower the net fresh use and the lower the terminal discharge. Consequently, in order to minimize the terminal discharge of the targeted species, we should recycle the maximum amount from terminal streams (or paths leading to terminal streams) to replace fresh feed. The maximum recyclable load of the targeted species is the lower of the two loads: the fresh and the terminal, i.e.

$$R^{MAX} = \text{argmin}\ \{F^{AFR}, T^{AGMIN, AFR}\} \tag{2.4}$$

where argmin refers to the lowest value in the set of loads (in this case the fresh and terminal loads).

As a result of recycle, the fresh load after mass integration becomes

$$F^{AMI} = F^{AFR} - R^{MAX} \tag{2.5}$$

Therefore, the target for minimum discharge of the targeted species after mass integration (T^{AMI}) can be calculated through the following overall material balance after mass integration:

$$T^{AMI} = F^{AMI} + Net\_G^{MIN} \quad (2.6)$$

Alternatively, the target for minimum discharge can be calculated from a material balance around the recovery and recycle system:

$$T^{AMI} = T^{AGMIN,\,AFR} - R^{MAX} \quad (2.7)$$

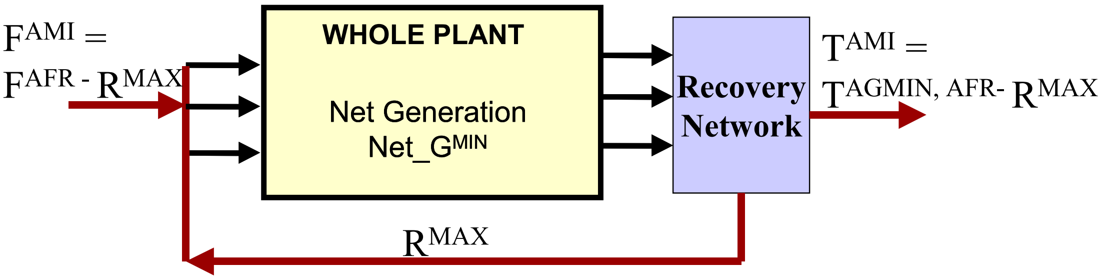

Fig. 2.4. Targeting for Minimum Discharge of Targeted Species

It is worth mentioning that in the spirit of targeting, it is not necessary to determine the type or techno-economic details of the recovery system. The objective is to determine the target for minimum load to be discharged from the plant. Later, we will discuss how the various alternatives are systematically screened with the objective of meeting this target at minimum cost.

The foregoing procedure can be summarized by the flowchart shown in Fig. 2.5. First, generation and depletion information are gathered as data or models. These include information on the depletion or generation of the targeted species through chemical reactions, non-point loss of the species through fugitive emissions or leaks, etc. Data are also collected on the amount of the targeted species in fresh feeds entering the process or terminal streams leaving the process. The net generation is first minimized. Then, the fresh feed of the targeted species is minimized by adjusting design and operating variables. Next, a recovery system is placed to recover maximum recyclable load (the lower of fresh and terminal loads). Hence, the fresh feed is minimized as maximum recycle is used to replace fresh feed. Finally, an overall material balance is used to calculated the target for minimum waste discharge.

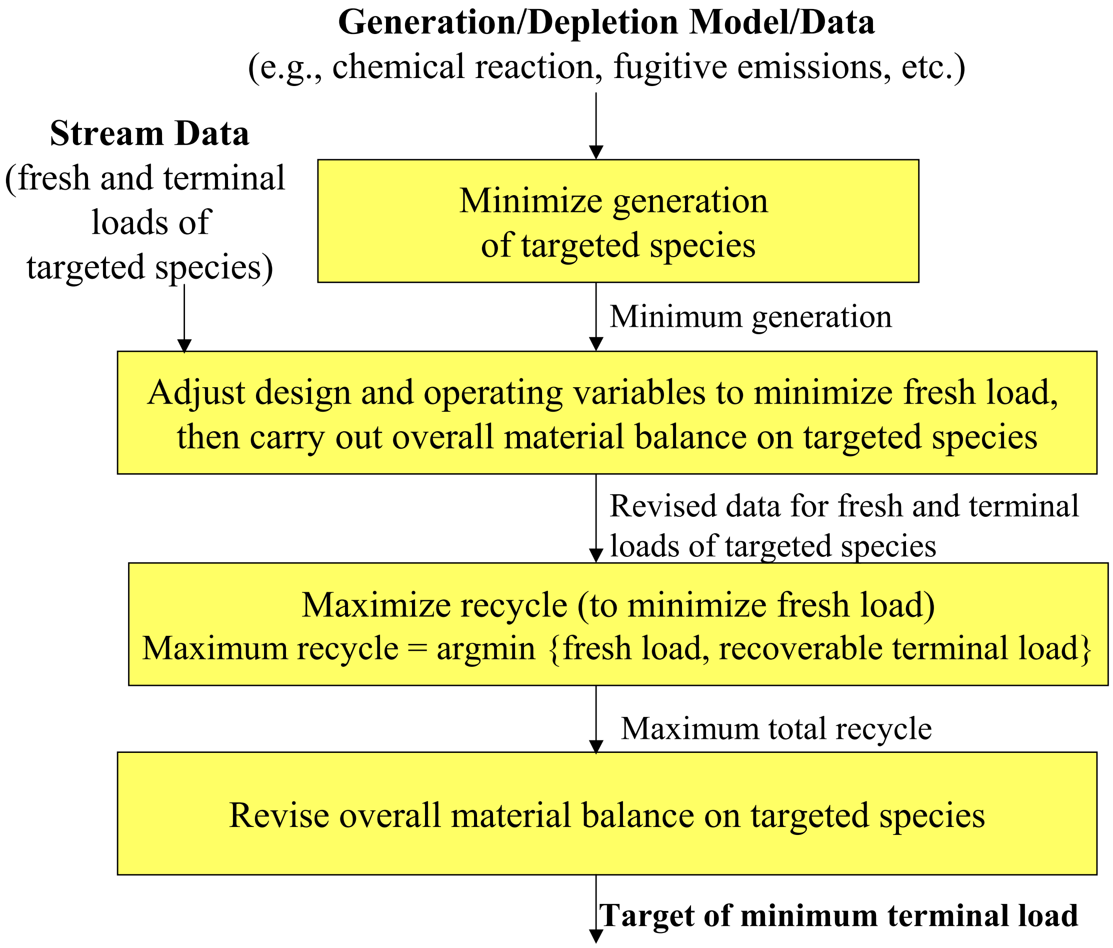

Fig. 2.5. Procedure for Identifying Minimum Waste Discharge

TARGETING FOR MINIMUM PURCHASE OF FRESH MATERIAL UTILITIES

We now move to the case of targeting minimum fresh usage of materials utilities (e.g, water, solvents, additives, etc.). The overall material balance can be written as:

$$F^{BMI} = T^{BMI} - Net\_G^{BMI} \tag{2.8}$$

For the special case, when the net generation is independent of stream recycle and adjustments in fresh feed, we can use a procedure similar to the one described for minimum waste discharge. The key difference is that the net generation of the targeted species is maximized (as opposed to minimized in the case of waste discharge). This can be deduced from the overall material balance given by Eq. 2.8 which entails maximizing the net generation in order to minimizing the fresh load. The targeting scheme is shown in Fig. 2.6.

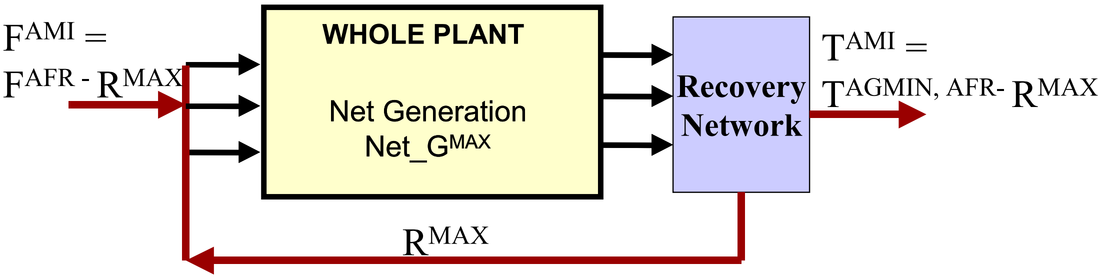

Fig. 2.6. Targeting for Minimum Usage of Material Utilities

It is worth pointing out that when the net generation is not to be altered, the target procedures for minimizing waste discharge and fresh usage become identical. Other objectives such as minimizing raw materials and maximizing yield can be similarly developed (e.g., Al-Otaibi and El-Halwagi, 2004).

MASS-INTEGRATION STRATEGIES FOR ATTAINING TARGETS

Once a target is determined, it is necessary to develop cost-effective strategies to reach the target. In general, these strategies include stream segregation/mixing, recycle, interception using separation devices, changes in design and operating conditions of units, materials substitution, and technology changes including the use of alternate chemical pathways. These strategies can be classified into a hierarchy of three categories (El-Halwagi, 1999; Noureldin and El-Halwagi, 2000):

- No/Low Cost Changes
- Moderate Cost Modifications, and
- New Technologies

Three main factors can be used in describing these strategies, economics, impact, and acceptability. The economic dimension can be assessed by a variety of criteria such as capital cost, return on investment, net present worth, and payback period. Impact is a measure of the effectiveness of the proposed solution in reducing negative ecological and hazard consequences of the process such as reduction in emissions and effluents from the plant. Acceptability is a measure of the likelihood of a proposed strategy to be accepted and implemented by the plant. In addition to cost, acceptability depends upon several factors including corporate culture, dependability, safety, and operability. Figure 2.7 is a schematic representation of the typical hierarchy of mass-integration strategies. These strategies are typically in ascending order of cost and impact and in descending order of acceptability.

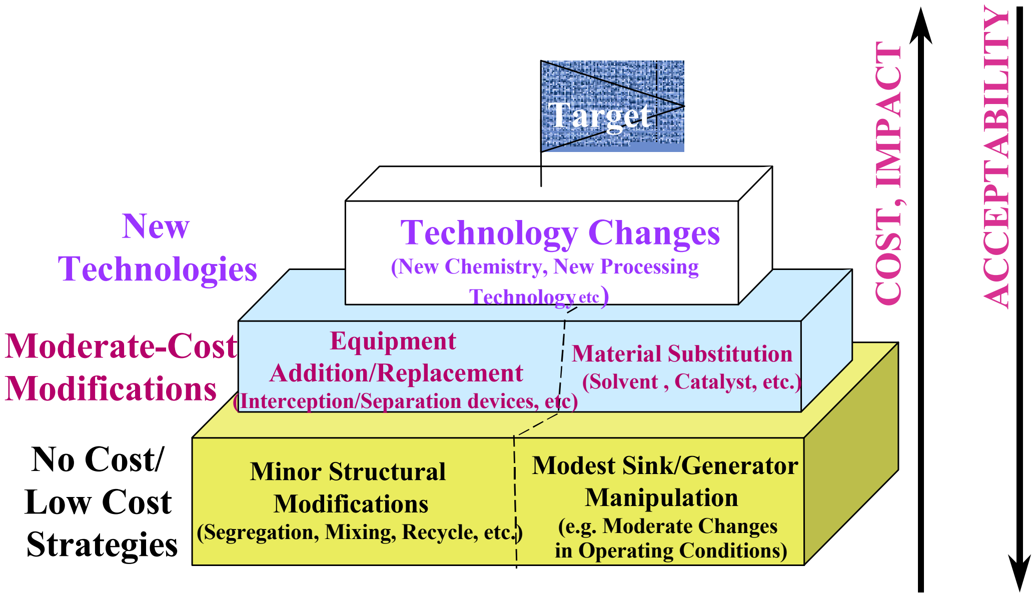

Fig. 2.7. Hierarchy of Mass-Integration Strategies
(El-Halwagi, 1999)

The development of process-related mass integration strategies will be covered throughout this book..

EXAMPLE 2.1: REDUCTION OF ACETIC ACID FRESH USAGE AND TERMINAL LOSSES IN A VINYL ACETATE PLANT

Vinyl acetate monomer “VAM” is manufactured by reacting acetic acid with oxygen and ethylene according to the following chemical reaction:

$C_2H_4 \quad + \quad 0.5\ O_2 \quad + \quad C_2H_4O_2 \quad = \quad C_4H_6O_2 \quad + \quad H_20$
Ethylene Oxygen Acetic Acid VAM Water

Consider the process shown in Fig. 2.8. A fresh feed of 10,000 kg/hr of acetic acid “AA” along with 200 kg/hr of water are evaporated in an acid tower. The vapor is fed with oxygen and ethylene to the reactor where 7,000 kg/hr of acetic acid are reacted and 10,000 kg/hr of VAM are formed. The reactor off gas is cooled and fed to first absorber where AA (5,100 kg/hr) is used as a solvent. Almost all the gases leave from the top of the first absorption column together with 1,200 kg/hr of AA. This stream is fed to the second absorption column where water (200 kg/hr) is used to scrub acetic acid. The bottom product of the first absorption column is fed to the primary distillation tower where VAM is recovered as a top product (10,000 kg/hr) along with 200 kg/hr of water and a small amount of AA (100 kg/hr) which is not economically-justifiable to recover. This stream is sent to final finishing. The bottom product of the primary tower (6,800 kg/hr of AA and 2,300 kg/hr of water) is mixed with the bottom product of the second absorption column (1,200 kg/hr of AA and 200 kg/hr of water). The mixed waste is fed to a neutralization system followed by biotreatment. In this example, let us consider the case when no changes are made to the consumption by chemical reaction and there are no adjustments in design or operating conditions to reduce fresh AA consumption. What is the target for minimum fresh usage and minimum terminal losses of AA?

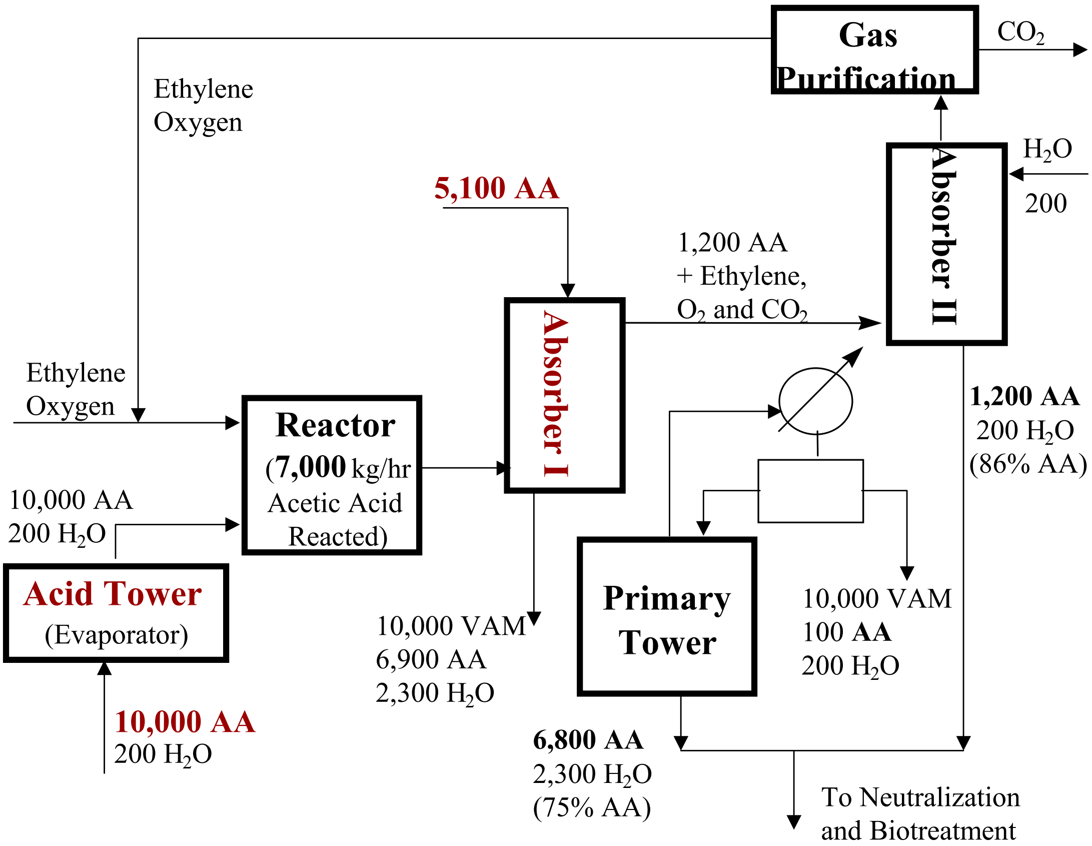

Fig. 2.8. VAM Production Process

Solution:

First, we extract the pertinent information regarding the fresh and terminal loads as well as consumption by chemical reaction. The data are presented in Fig. 2.9. Clearly, a net consumption of 7,000 kg AA/hr is the equivalent of –7,000 kg AA/hr of net generation. Since there are allowable changes in reaction or design and operating conditions affecting fresh consumption, we resort to recovery from terminal streams, recycle, and replacement of fresh AA. It is worth noting that the recoverable load from the terminal streams (8,000 kg AA/hr) is less than the fresh load (15,100 kg AA/hr). Hence, R^{MAX} is 8,000 kg AA/hr. Therefore, according to Eq. 2.5, we get a target for minimum fresh usage to be:

$$F^{AMI} = 15{,}100 - 8{,}000 = 7{,}100 \text{ kg AA/hr} \qquad (2.9)$$

Consequently, as can be seen from Fig. 2.10 the target for minimum terminal losses of AA is 100 kg AA/hr.

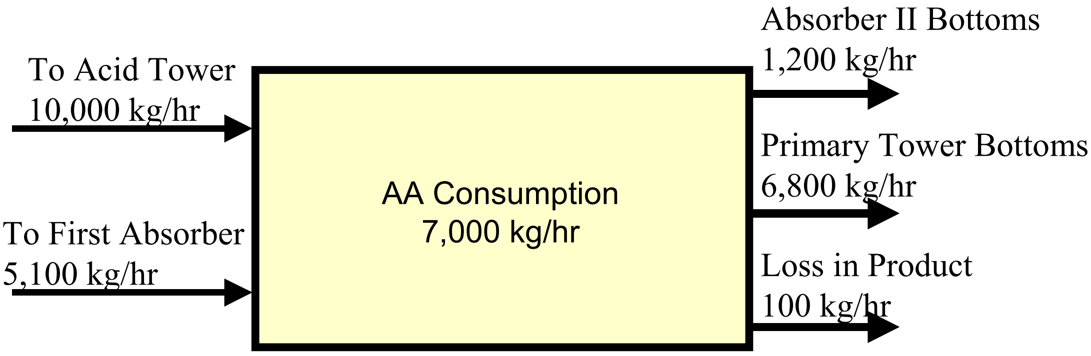

Fig. 2.9. Overall AA Material Balance for the VAM Process Before Mass Integration

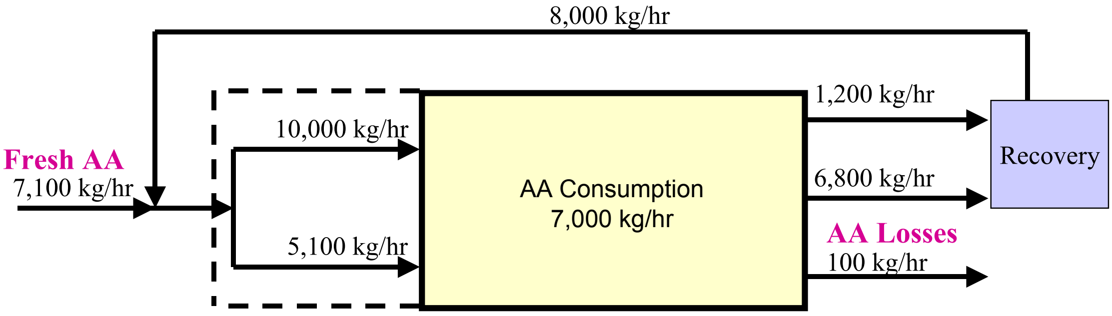

Fig. 2.10. Overall AA Material Balance for the VAM Process After Mass Integration

EXAMPLE 2.2: REDUCTION OF DISCHARGE IN A TIRE-TO-FUEL PLANT

This case study is adapted from El-Halwagi (1997) and Noureldin and El-Halwagi (2000). It involves a processing facility that converts scrap tires into fuel via pyrolysis. Figure 2.11 is a simplified flowsheet of the process. The discarded tires are fed to a high-temperature reactor where hydrocarbon content of the tires are broken down into oils and gaseous fuels. The oils are further processed and separated to yield transportation fuels. As a result of the pyrolysis reactions, water is formed. The amount of generated water is a function of the reaction temperature, T_{rxn}, through the following correlation:

$$W_{rxn} = 0.152 + (5.37 - 7.84 \times 10^{-3}\, T_{rxn})\, e^{(27.4 - 0.04 T_{rxn})} \qquad (2.10)$$

Where W_{rxn} is in kg/s and T_{rxn} is in K. At present, the reactor is operated at 690 K which leads to the generation of 0.12 kg water/s. In order to maintain acceptable product quality, the reaction temperature should be maintained within the following range:

$$690 \le T_{rxn}(K) \le 740 \qquad (2.11)$$

The gases leaving the reactor are passed through a cooling/condensation system to recover some of the light oils. In order to separate the oils, a decanter is used to separate the mixture into two layers: aqueous and organic. The aqueous layer is a wastewater stream whose flowrate is designated as W_1 and it contains phenol as the primary pollutant. The organic layer is mixed with the liquid products of the reactor and fed to finishing. As a result of fuel finishing, a gaseous waste is produced and flared. As a safety precaution to prevent the back-propagation of fire from the flare, a seal pot (or a water valve) is placed before the flare to provide a buffer zone between the fire and the flare gas. The flowrate of the water stream passing through the seal pot is referred to as G_2 and an equivalent flowrate of wastewater stream, $W_2 = G_2$, is withdrawn from the seal pot.

Tire shredding is achieved by using high-pressure water jets. The shredded tires are fed to the process while the spent water is filtered. The wet cake collected from the filtration system is forwarded to solid waste handling. The filtrate is mixed with fresh water-jet makeup "G_1" to compensate for water losses with the wet cake "W_3" and the shredded tires. The mixture of filtrate and water makeup is fed to a high-pressure compression station for recycle to the shredding unit. The flowrate of water-jet makeup depends on the applied pressure coming out of the compression stage "P_{comp}" via the following expression:

$$G_1 = 0.47\, e^{-0.009\, P_{comp}} \qquad (2.12)$$

where G_1 is in kg/s and P_{comp} is in atm. In order to achieve acceptable shredding, the jet pressure may be varied within the following range:

$$70 \le P_{comp}(atm) \le 90 \qquad (2.13)$$

At present, P_{comp} is 70 atm which requires a water-jet make-up flowrate of 0.25 kg/s.
The water lost in the cake is related to the mass flowrate of the water-jet makeup through:

$$W_3 = 0.4\, G_1 \qquad (2.14)$$

In addition to the water in the wet cake, the plant has two primary sources for wastewater; from the decanter (W_1) and from the seal pot (W_2). At present, the values of W_1, W_2, and W_3 are 0.27, 0.15, and 0.10 kg/s, respectively. The wastewater from the decanter contains about 500 ppm of phenol. Within the range of allowable operating changes, this concentration can be assumed to remain constant. At present, the wastewater from the seal pot contains no phenol. The plant has been shipping the wastewater streams W_1 and W_2 for off-site treatment. The cost of wastewater transportation and treatment is \$0.10/kg leading to a wastewater treatment cost of approximately \$ 1.33 million/yr. W_3 has been processed on site. Because of the characteristics of W_3, the plant does not allow its recycle back to the process even after waste-handling processing. The plant wishes to reduce off-site treatment of wastewater streams W_1 and W_2 to avoid cost of off-site treatment and alleviate legal-liability concerns in case of transportation accidents or inadequate treatment of the wastewater. The objective of this problem is determine a target for reduction in flowrate of terminal discharges W_1 and W_2.

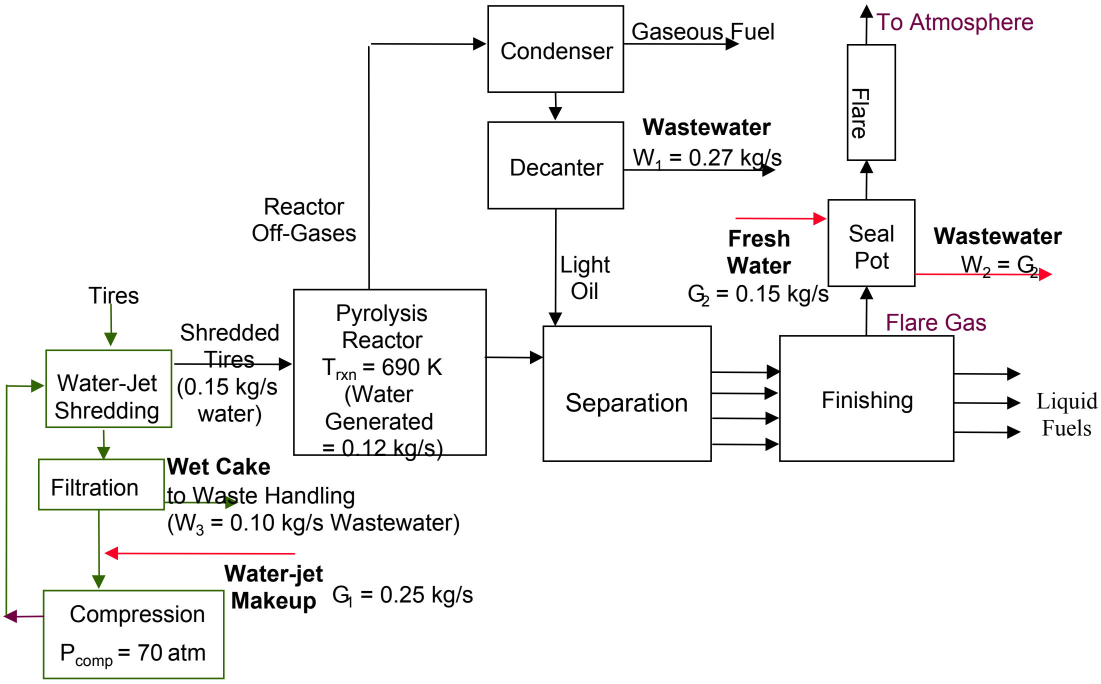

Fig. 2.11 Simplified Flowsheet of Tire-to-Fuel Plant

SOLUTION

Figure 2.12 shows an overall water balance for the process before mass integration.

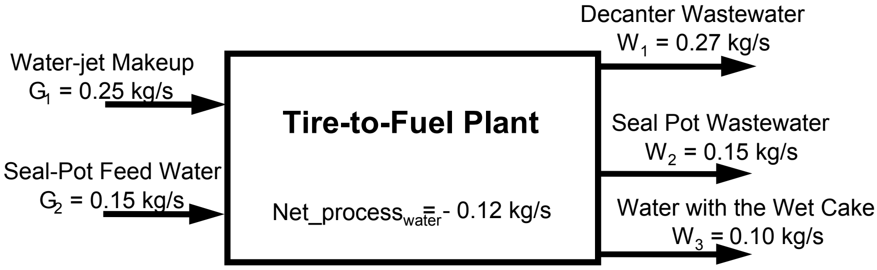

Fig. 2.12 Overall Water Balance for the Tire-to-Fuel Process

The first step in the analysis is to reduce the terminal discharge by minimizing the net generation of water. Figure 2.13 is a graphical representation of Eq. (2.10) illustrating the net generation of water through chemical reaction as a function of the reaction temperature. As can be seen from this graph, the minimum generation of water is 0.08 kg/s and is attained at a reaction temperature of 710 K.

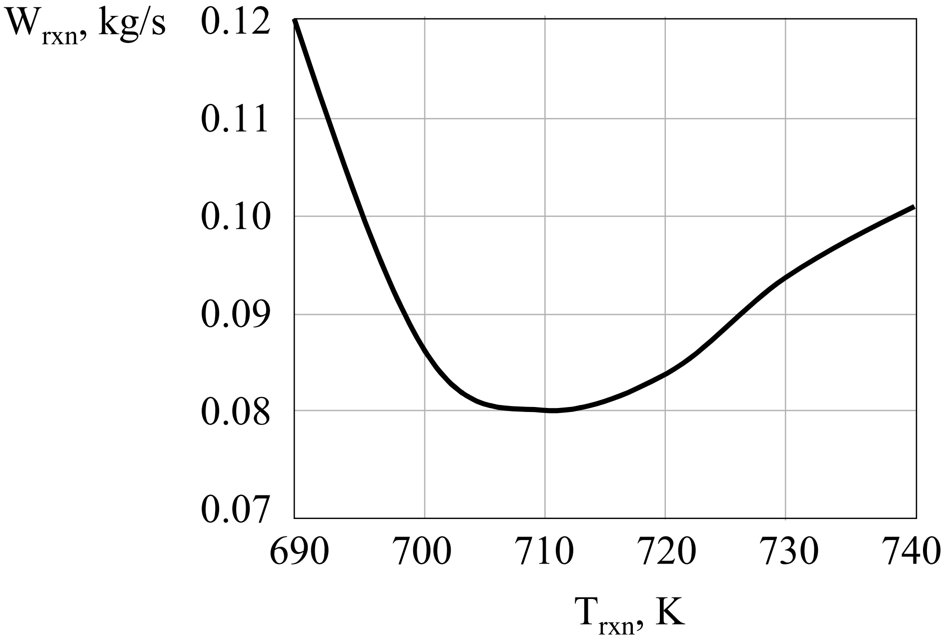

Fig. 2.13. Rate of Water Consumption as a Function of Reaction Temperature

Next, we adjust design and operating parameters so as to minimize fresh water consumption. As mentioned earlier, the fresh water used in shredding is a function of pressure as given by Eq. 2.12:

$G_1 = 0.47\ e^{-0.009\ P_{comp}}$ (2.12)

where P_{comp} should be maintained within a permissible interval of [70atm , 95 atm]. Therefore, in order to minimize the fresh water needed for shredding, the value of P_{comp} should be set to its maximum limit of 95 atm. Consequently, G_1 is reduced to 0.20 kg/s. According to Eq. (2.14), the new value of W_3 is given by:

$W_3 = 0.4*0.20 = 0.08$ kg/s (2.15)

With the new values of G_1 and W_3 and with the water generation minimized to 0.08 kg/s, an overall water balance provides the value of W_2 to be 0.15 kg/s. These results are shown in Fig. 10 and represent the overall water balance after sink/generator manipulation with existing units and current process configuration. Next, we calculate the target for water usage and discharge using interception (cleaning up of recycled water) and recycle. This targeting analysis is shown in Fig. 2.15 and it yields a target of zero fresh water and 0.08 kg/s for wastewater discharge.

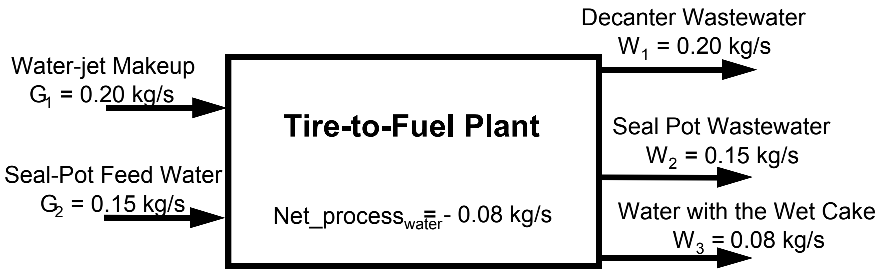

Fig. 2.14 Overall Water Balance after Sink/Generator Manipulation

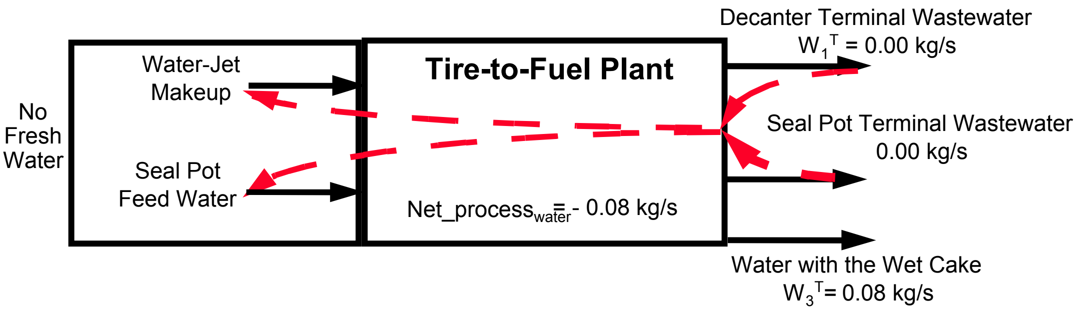

Fig. 2.15 Targeting for Minimum Water Usage and Discharge

HOMEWORK

2.1. Consider the VAM process described in Example 2.1. A new reaction pathway has been developed and will to be used for the production of VAM. This new reaction does not involve acetic acid. The rest of the process remains virtually unchanged and the AA losses with the product are 100 kh/hr. What are the targets for minimum fresh usage and discharge/losses of AA?

2.2. Consider the magnetic-tape manufacturing process shown by Fig. 2.16. In this process (Dunn et al., 1995, El-Halwagi, 1997), coating ingredients are dissolved in 0.09 kg/s of organic solvent and mixed to form a slurry. The slurry is suspended with resin binders and special additives. Next, the coating slurry is deposited on a base film. Nitrogen gas is used to induce evaporation rate of solvent that is proper for deposition. In the coating chamber, 0.011 kg/s of solvent are decomposed into other organic species. The decomposed organics are separated from the exhaust gas in a membrane unit. The retentate stream leaving the membrane unit has a flowrate of 3.0 kg/s and is primarily composed of nitrogen that is laden with 1.9 wt/wt% of the organic solvent. The coated film is passed to a dryer where nitrogen gas is employed to evaporate the remaining solvent. The exhaust gas leaving the dryer has a flowrate of 5.5 kg/s and contains 0.4 wt/wt% solvent. The two exhaust gases are mixed and disposed off.

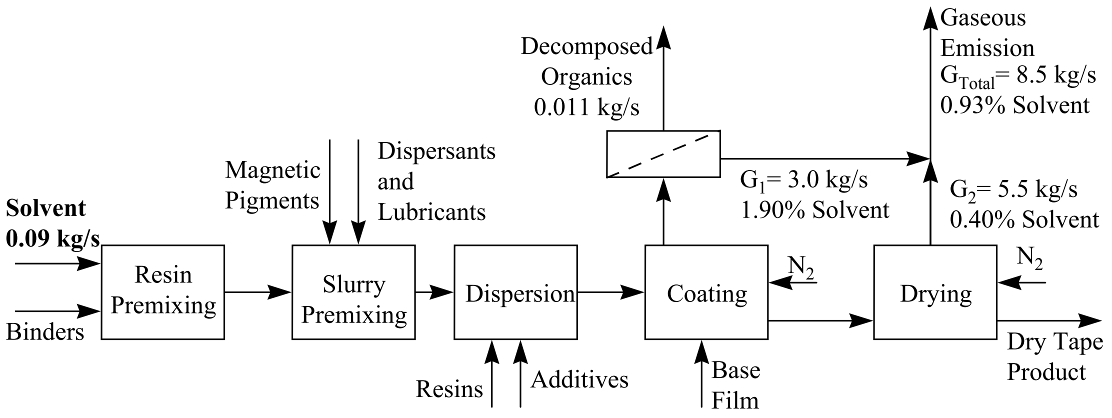

Fig. 2.16. Magnetic Tape Plant (Dunn et al., 1995; El-Halwagi, 1997)

In addition to the environmental problem, the facility is concerned about the waste of resources, primarily in the form of used solvent (0.09 kg/s) that costs about $2.3 million/yr. It is desired to undertake a mass-integration analysis to optimize solvent usage, recovery and losses. Determine the target for minimizing fresh solvent usage in the process.

2.3. Every year, significant quantities of plastic wastes are disposed of to landfills. An emerging processing technique for reclaiming plastic waste is to convert it into liquid fuels. A schematic process flowsheet is given by Fig. 2.17. The data in this problem are taken from Hamad and El-Halwagi (1998).

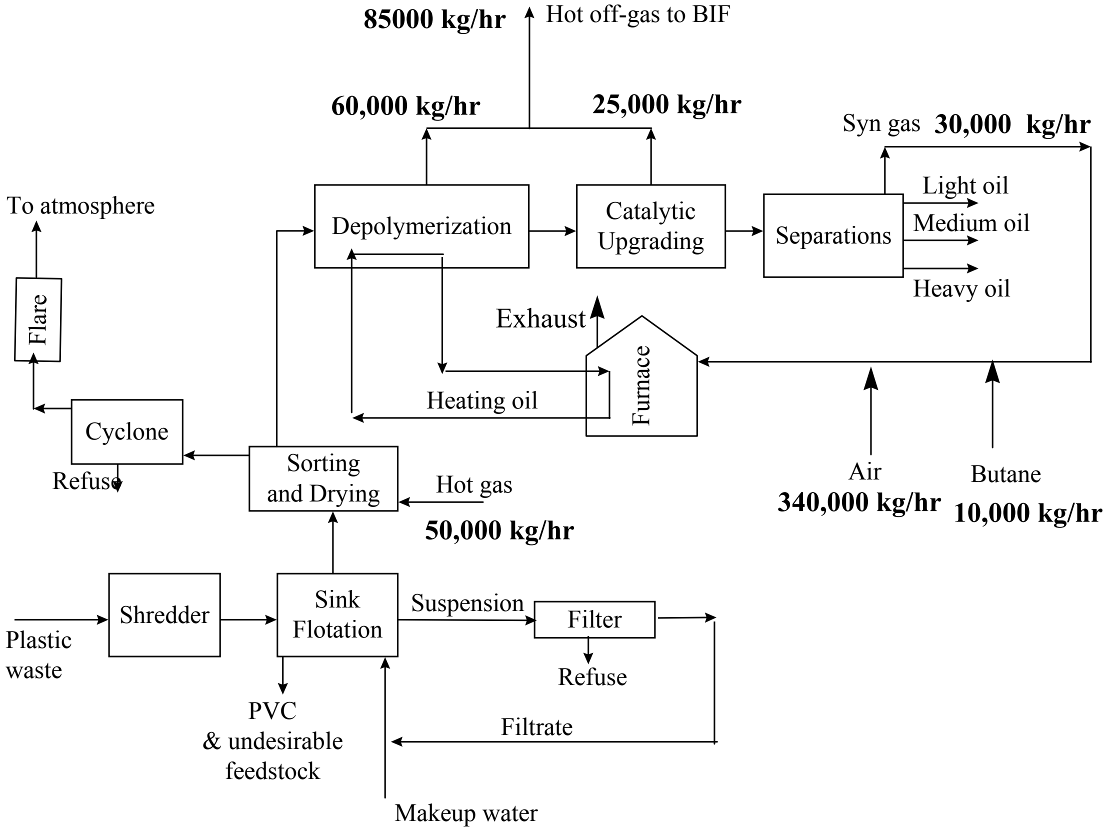

Fig. 2.17 A Simplified Plant for Oil Production from Waste Plastic (Hamad and El-Halwagi, 1998)

Plastic waste (feedstock) is first shredded then sorted in a sink/flotation unit to remove polyvinyl chloride (PVC) and undesirable feedstock. The suspension from the sink floatation unit is filtered. The refuse from filtration is rejected and the filtrate is recycled to the sink flotation unit. The remaining feedstock is sorted and dried using 50,000 kg/hr of hot gas. At present, this hot gas contains no butane. Also, no butane is formed in sorting and drying. The hot gas leaving the sorting and drying process is passed through a cyclone to remove suspended solids as refuse. The cyclone is followed by a flare where any organics are burned.

The sorted/dried feedstock enters a depolymerization unit where a butane-laden gaseous stream (total flowrate of gas is 60,000 kg/hr and it contains 7,200 ppmw butane) is generated. The slurry leaving the depolymerization unit is upgraded in a catalytic unit then separated into various hydrocarbon cuts. The off-gas leaving the catalytic upgrading unit has a flowrate of 25,000 kg/hr and contains 80,000 ppmw of butane.

The depolymerization unit is heated using a recirculating heating oil coming from a furnace. The feed to the furnace consists of 30,000 kg/hr of syngas (composed primarily of butane), 10,000 kg/hr of butane, and 340,000 kg/hr of air. The exhaust from the furnace contains almost no butane.

Until recently, the gaseous streams from the depolymerization and catalytic units were mixed and fed to a boiler/industrial furnace (BIF). Due to economic, safety and environmental concerns the BIF operation is to be discontinued and the mixed off-gas is to be rerouted in the plant.

a. What is current flowrate (kg/hr) of purchasd fresh butane?
b. What is the total amount (kg/hr) of butane generated by chemical reaction in the process? Hint: butane generation by chemical reaction takes place in the depolymerization and catalytic upgrading units

c. How much (kg/hr) butane is depleted by chemical reaction in the process? Hint: butane depletion by chemical reaction takes place in the furnace.

d. What is the target (kg/hr) for minimum purchase of fresh butane?

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