Chapter 5. Tracing Chemicals through the Process Flow Diagram

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What You Will Learn

- In a continuous chemical process, there are reactants, products, and inerts.
- These components enter, leave, are formed, or are consumed in the process.
- Each component can be followed through the process.

In Chapter 2, the unit operations from a PFD were classified into one of the six blocks of a generic block flow process diagram. In this chapter, you gain a deeper understanding of a chemical process by learning how to trace the paths taken by chemical species through a chemical process.

5.1. Guidelines and Tactics for Tracing Chemicals

In this chapter, guidelines and some useful tactics are provided to help you trace chemicals through a process. Two important operations for tracing chemical pathways in PFDs are the adiabatic mixer and adiabatic splitter.

Mixer: Two or more input streams are combined to form a single stream. This single output stream has a well-defined composition, phase(s), pressure, and temperature.

Splitter: A single input stream is split into two or more output streams with the same temperature, pressure, and composition as the input stream. All streams involved differ only in flowrate.

These operations are found where streams meet or a stream divides on a PFD. They are little more than tees in pipelines in the plant. These operations involve little design and minimal cost. Hence, they are not important in estimating the capital cost of a plant and would not appear on a list of major equipment. However, you will find in Chapter 13 that these units are included in the design of flowsheets for implementing and using chemical process simulators.

The mixers and splitters are highlighted as shaded boxes on the flow diagrams presented in this chapter. They carry an “m” and “s” designation, respectively.

5.2. Tracing Primary Paths Taken by Chemicals in a Chemical Process

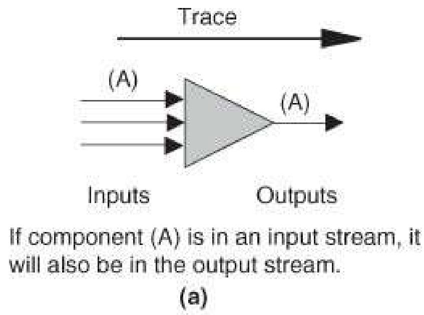
Chemical species identified in the overall block flow process diagram (those associated with chemical reactions) are termed **primary chemicals.** The paths followed by primary chemicals between the reactor and the boundaries of the process are termed **primary flow paths.** Two general guidelines should be followed when tracing these primary chemicals:

1. **Reactants:** Start with the feed (left-hand side of the PFD) and trace chemicals forward toward the reactor.
2. **Products:** Start with the product (right-hand side of the PFD) and trace chemicals backward toward the reactor.

The following tactics for tracing chemicals apply to all unit operations *except for* chemical reactors:

Tactic 1: Any unit operation, or group of operations, that has a single or multiple input streams and a single output stream is traced in a forward direction. If chemical A is present in any input stream, it must appear in the single output stream (see Figure 5.1[a]).

Tactic 2: Any unit operation, or group of operations, that has a single input stream and single or multiple output streams is traced in a backward direction. If chemical A is present in any output stream, it must appear in the single input stream (see Figure 5.1[b]).



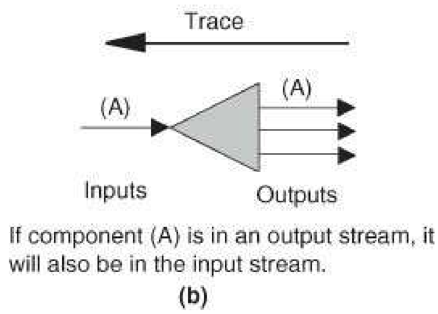


Figure 5.1. Tactics for Tracing Chemical Species

Tactic 3: Systems such as distillation columns are composed of multiple unit operations with a single input or output stream. It is sometimes necessary to consider such equipment combinations as blocks before implementing Tactics 1 and 2.

When tracing chemicals through a PFD, it is important to remember the following:

Only in reactors are feed chemicals transformed into product chemicals.

You may occasionally encounter situations where both reactions and physical separations take place in a single piece of equipment. In most cases, this is undesirable but unavoidable. In such situations, it will be necessary to divide the unit into two imaginary, or phantom, units. The chemical reactions take place in one phantom unit, and the separation in the second phantom unit. These phantom units are never shown on the PFD, but such units are useful when building a flowsheet for a chemical process simulator (see Chapter 13).

These guidelines are demonstrated in Example 5.1, by determining the paths of the primary chemicals in the toluene hydrodealkylation process. The only information used is that provided in the skeleton process flow diagram given in Figure 1.3.

Example 5.1.

For the toluene hydrodealkylation process, establish the primary flow pathway for

a. Toluene between the feed (Stream 1) and the reactor
b. Benzene between the reactor and the product (Stream 15)

Hint: Consider only one unit of the system at a time. Refer to Figure E5.1.

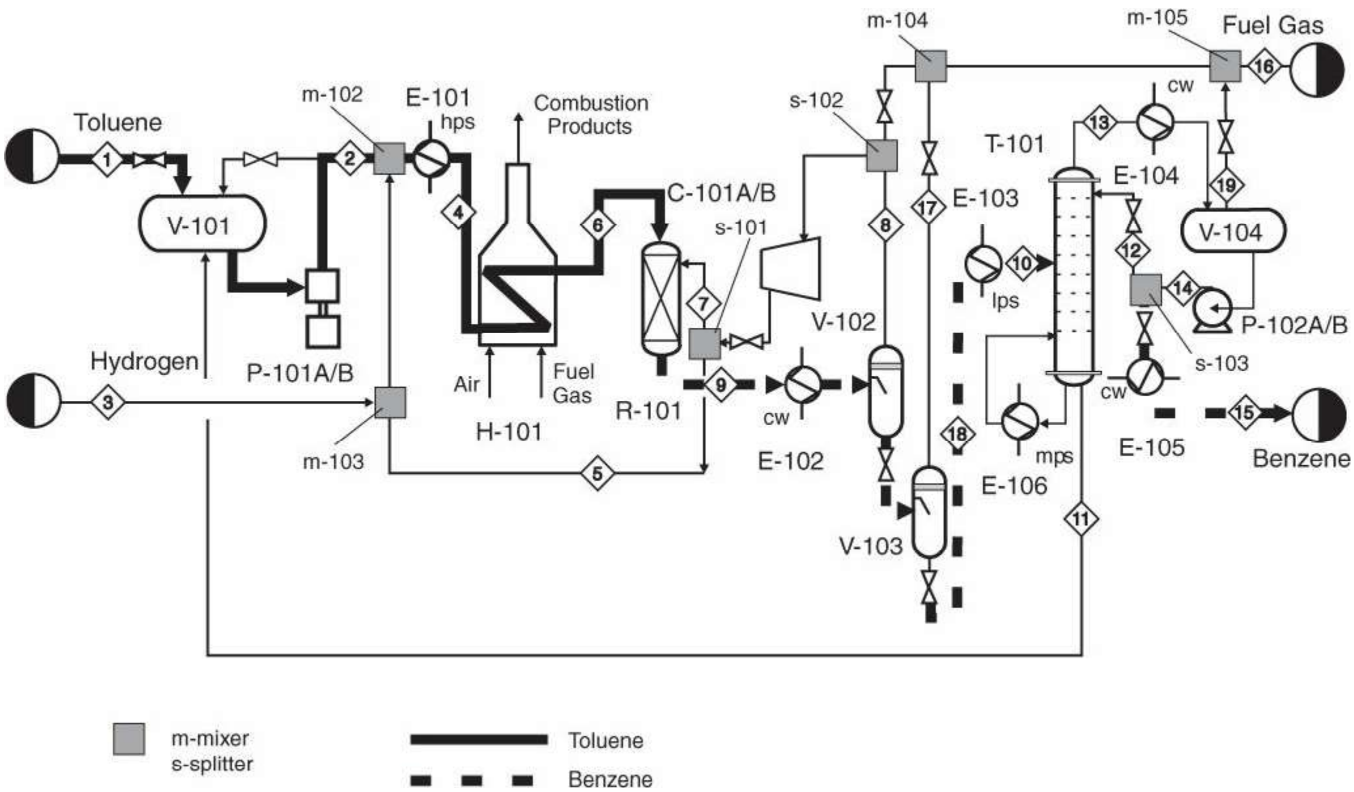


Figure E5.1. Primary Chemical Pathways for Benzene and Toluene in the Toluene Hydrodealkylation Process (Figure 1.3)

Toluene Feed: Tactic 1 is applied to each unit operation in succession.

a. Toluene feed Stream 1 mixes with Stream 11 in V-101. A single unidentified stream leaves tank V-101 and goes to pump P-101. All the toluene feed is in this stream.

b. Stream 2 leaves pump P-101 and goes to mixer m-102. All the feed toluene is in this stream.

c. A single unidentified stream leaves mixer m-102 and goes to exchanger E-101. All the feed toluene is in this stream.

d. Stream 4 leaves exchanger E-101 and goes to heater H-101. All the feed toluene is in this stream.

e. Stream 6 leaves heater H-101 and goes to reactor R-101. All the feed toluene is in this stream.

Benzene Product: Tactic 2 is applied to each unit operation in succession.

a. Product Stream 15 leaves exchanger E-105.

b. Entering exchanger E-105 is an undesignated stream from s-103 of the distillation system. It contains all of the benzene product.

c. Apply Tactic 3 and treat the tower T-101, pump P-102, exchangers E-104 and E-106, vessel V-104, and splitter s-103 as a system.

d. Entering this distillation unit system is Stream 10 from exchanger E-103. It contains all the benzene product.

e. Entering exchanger E-103 is Stream 18 from vessel V-103. It contains all the benzene product.

f. Entering vessel V-103 is an undesignated stream from vessel V-102. It contains all the benzene product.

g. Entering vessel V-102 is an undesignated stream from exchanger E-102. It contains all the benzene product.

h. Entering exchanger E-102 is Stream 9 from reactor R-101. It contains all the benzene product.

The path for toluene was identified as an enhanced solid line in Example 5.1. For this case, it was not necessary to apply any additional information about the unit operations to establish this path. The two streams that joined the toluene path did not change the fact that all the feed toluene remained as part of the stream. All the toluene fed to the process in Stream 1 entered the reactor, and this path represents the primary path for toluene.

The path for benzene was identified as an enhanced dotted line in Example 5.1. The equipment that makes up the distillation system was considered as an operating system and treated as a single unit operation. The fact that, within this group of process units, some streams were split with some of the flow returning upstream did not change the fact that the product benzene always remained in the part of the stream that continued to flow toward the product discharge. All the benzene product followed this path, and it represents the primary path for the benzene. The flow path taken for the benzene through the distillation column section is shown in more detail in Figure 5.2. The concept of drawing envelopes around groups of equipment in order to carry out material and energy balances is introduced early into the chemical engineering curriculum. This concept is essentially the same as the one used here to trace the path of benzene through the distillation column. The only information needed about unit operations used in this analysis was the identification of the multiple units that made up the distillation system. This procedure can be used to trace chemicals throughout the PFD and forms an alternative tracing method that is illustrated in Example 5.2.

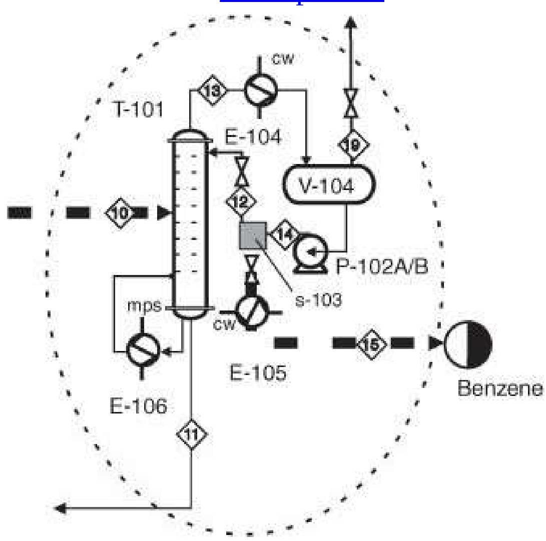


Figure 5.2. Envelope around Tower T-101 Showing Alternative Method for Tracing Benzene Stream

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Example 5.2.

Establish the primary flow pathway for

a. Hydrogen between its introduction as a feed and the reactor

b. Methane between its generation in the reactor and the discharge from the process as a product

In order to determine the primary flow paths, systems are developed (by drawing envelopes around equipment) that progressively include additional unit operations. Reference should be made to Figure

E5.2(a) for viewing and identifying systems for tracing hydrogen.

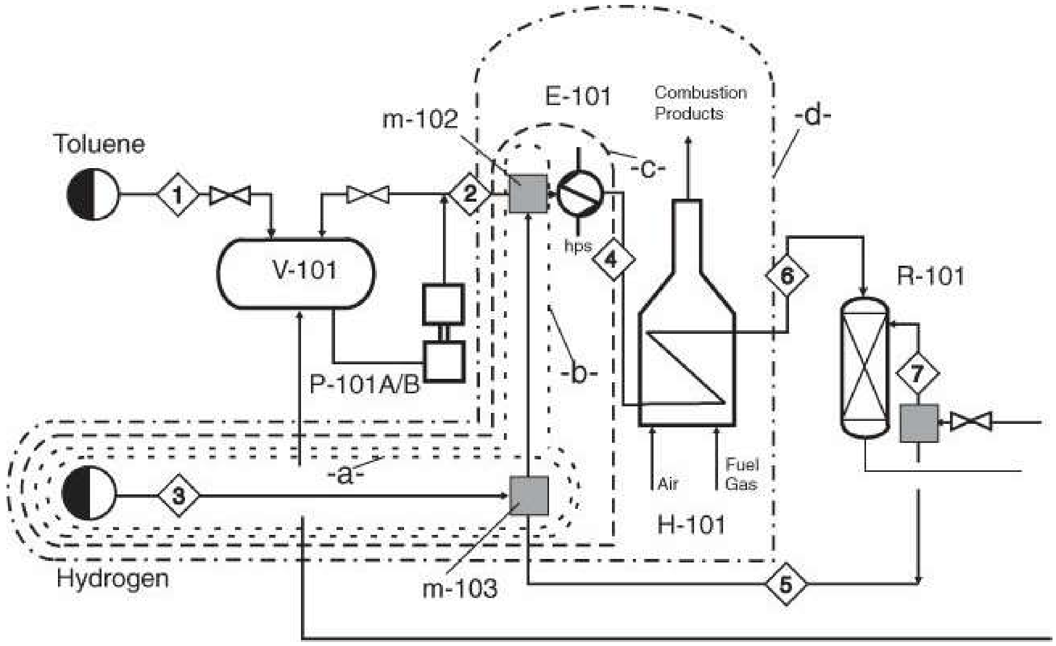

Figure E5.2(a). Tracing Primary Chemical Pathways Using the Envelope Method

Hydrogen Feed: Tactic 1 is applied to each system in a forward progression. Each system includes the hydrogen feed Stream 3, and the next piece of equipment to the right.

System -a-: This system illustrates the first step in our analysis. The system includes the first unit into which the hydrogen feed stream flows. The unidentified stream leaving mixer m-103 contains the feed hydrogen.

System -b-: Includes mixers m-103 and m-102. The exit stream for this system includes the feed hydrogen.

System -c-: Includes mixers m-103, m-102, and exchanger E-101. The exit stream for this system, Stream 4, includes the feed hydrogen.

System -d-: Includes mixers m-103, m-102, exchanger E-101, and heater H-101. The exit stream for this system, Stream 6, includes the feed hydrogen. Stream 6 goes to the reactor.

The four steps described above are illustrated in Figure E5.2(a). A similar analysis is possible for tracing methane, and the steps necessary to do this are illustrated in Figure E5.2(b). These steps are discussed briefly below.

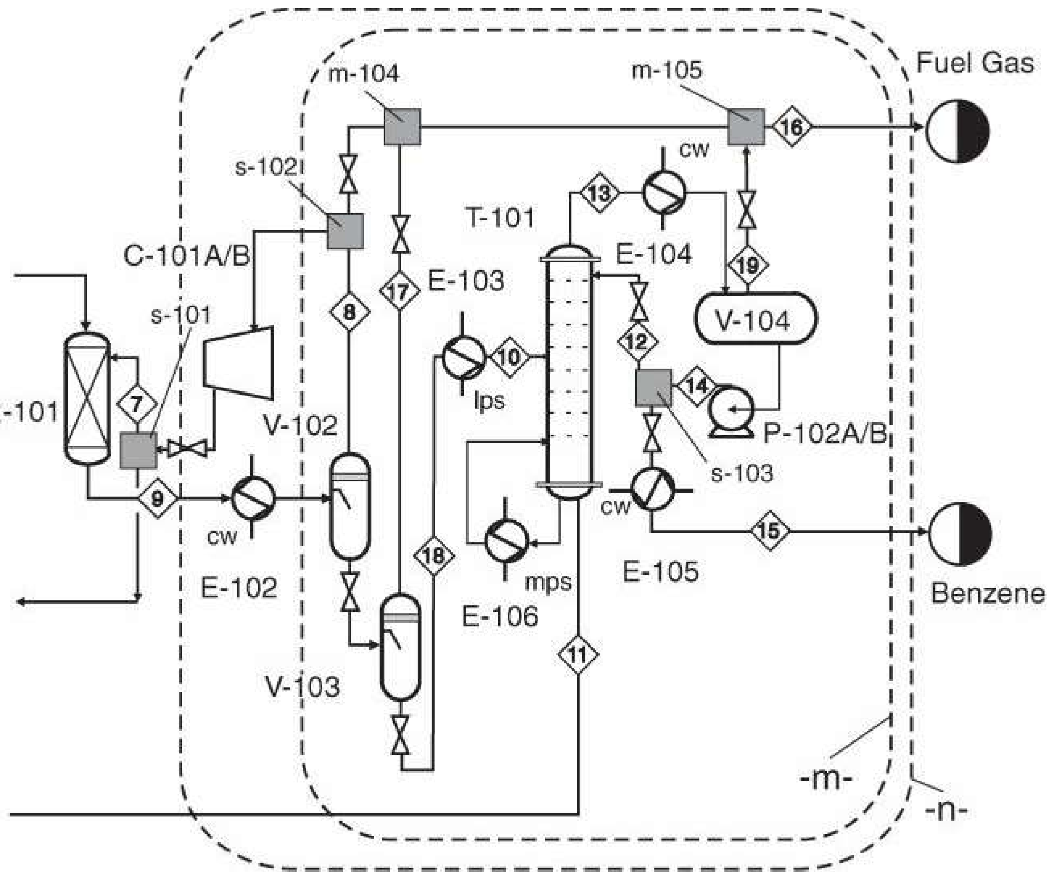

Figure E5.2(b). Tracing the Primary Flow Path for Methane in Toluene Hydrodealkylation PFD

Methane Product: The methane produced in the process leaves in the fuel gas, Stream 16. Tactic 2 is applied to each system containing the fuel gas product, in backward progression.

System -m-: Consists of m-105, m-104, E-105, T-101, V-104, P-102, s-103, E-104, E-106, E-103, V-102, V-103, and s-102. This is the smallest system that can be found that contains the fuel gas product stream and has a single input.

System -n-: Includes the system identified above plus exchanger E-102 and compressor C-101. The inlet to E-102 contains all the methane in the fuel stream. This is Stream 9, which leaves the reactor.

In the first step of tracing methane, including only m-105 was attempted. This unit had two input streams, and it was not possible to determine which of these streams carried the methane that made up the product stream. Thus, Tactic 2 could not be used. In order to move ahead, additional units were added to m-105 to create a system that had a single input stream. The resulting system, System -m-, has a single input, with the unidentified stream coming from exchanger E-102. An identical problem would arise if the procedure used in Example 5.1 were implemented. Figure 5.3 shows the primary paths for the hydrogen and methane.

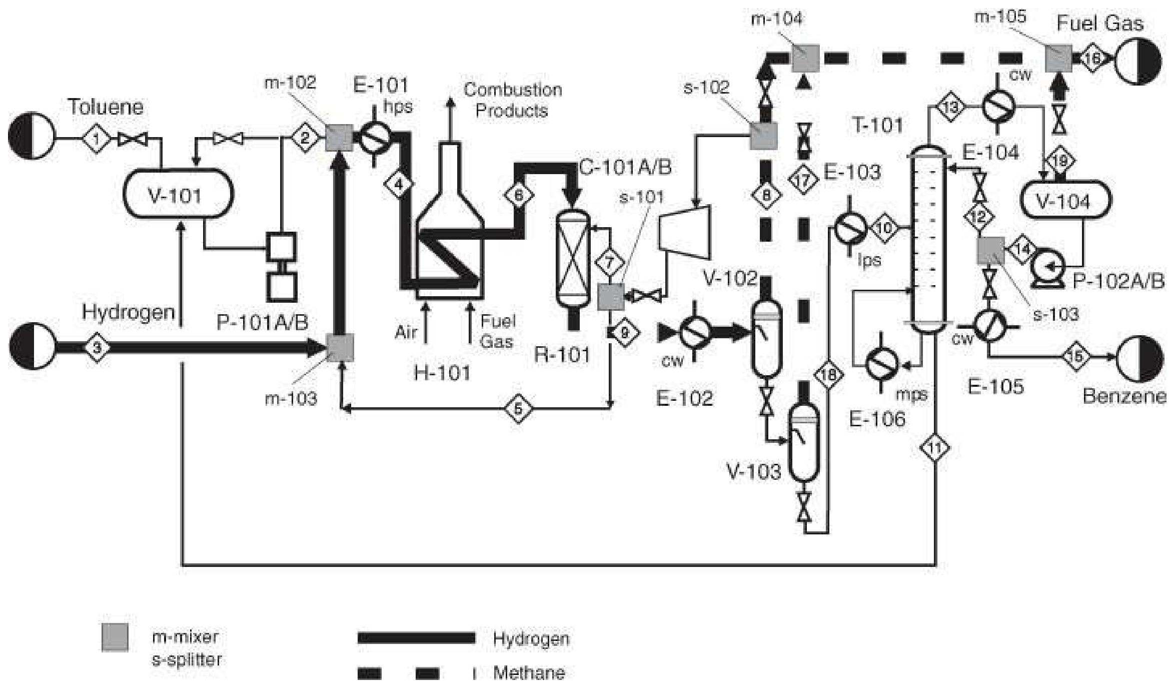

Figure 5.3. Primary Chemical Pathways for Methane and Hydrogen in the Toluene Hydrodealkylation PFD

5.3. Recycle and Bypass Streams

It is important to be able to recognize recycle and bypass streams in chemical processes. When identifying recycle and bypass streams, flow loops in the PFD are identified. Any time a flow loop is identified, either a recycle or a bypass stream exists. The direction of the streams, as indicated by the direction of the arrowheads, determines whether the loop contains a recycle or a bypass. The following tactics are applied to flow loops:

Tactic 4: If the streams in a loop flow so that the flow path forms a complete circuit back to the point of origin, then it is a **recycle loop.**

Tactic 5: If the streams in a loop flow so that the flow path does not form a complete circuit back to the place of origin, then it is a **bypass stream.**

It is worth noting that certain pieces of equipment normally contain recycle streams. In particular, distillation columns very often have top and bottoms product reflux streams, which are essentially recycle loops. When identifying recycle loops, which loops contain reflux streams and which do not can be determined easily. Example 5.3 illustrates the procedure for identifying recycle and bypass streams in the toluene hydrodealkylation PFD.

Example 5.3.

For the toluene hydrodealkylation PFD given in Figure E5.1, identify all recycle and bypass streams.

The recycle loops are identified in Figures E5.3(a) and E5.3(b). The main toluene recycle loop is highlighted in Figure E5.3(a), and the hydrogen recycle loops are shown in Figures E5.3(b)(a) and E5.3(b)(b). There are two reflux loops associated with T-101, and these are shown in Figures E5.3(b)(c) and E5.3(b)(d). Finally, there is a second toluene recycle loop identified in Figure E5.3(b)(e).

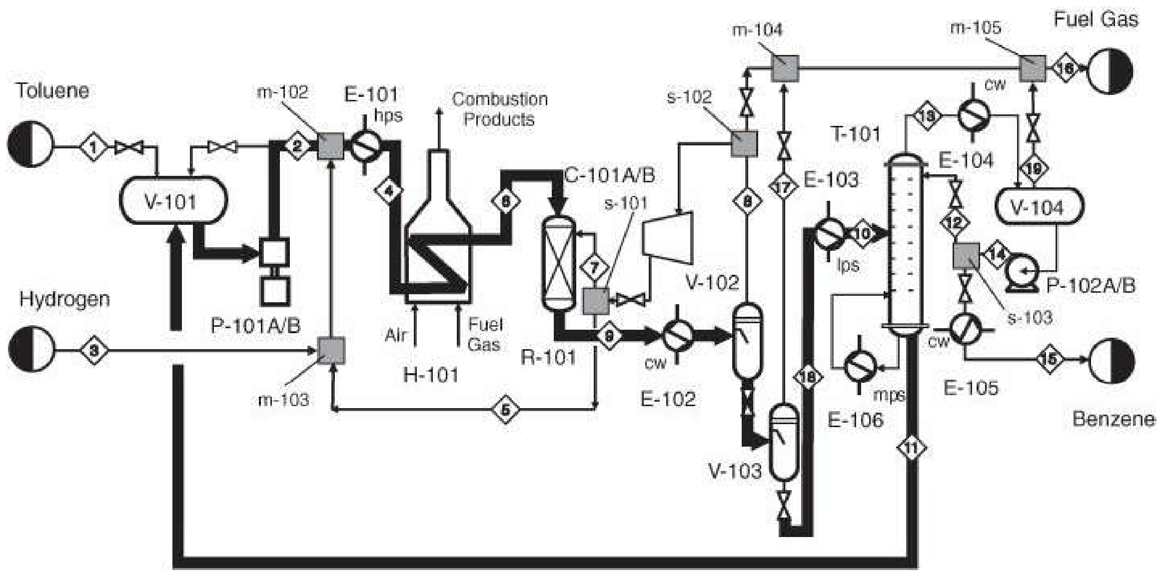

Figure E5.3(a). Identification of Toluene Recycle Loop in Toluene Hydrodealkylation PFD

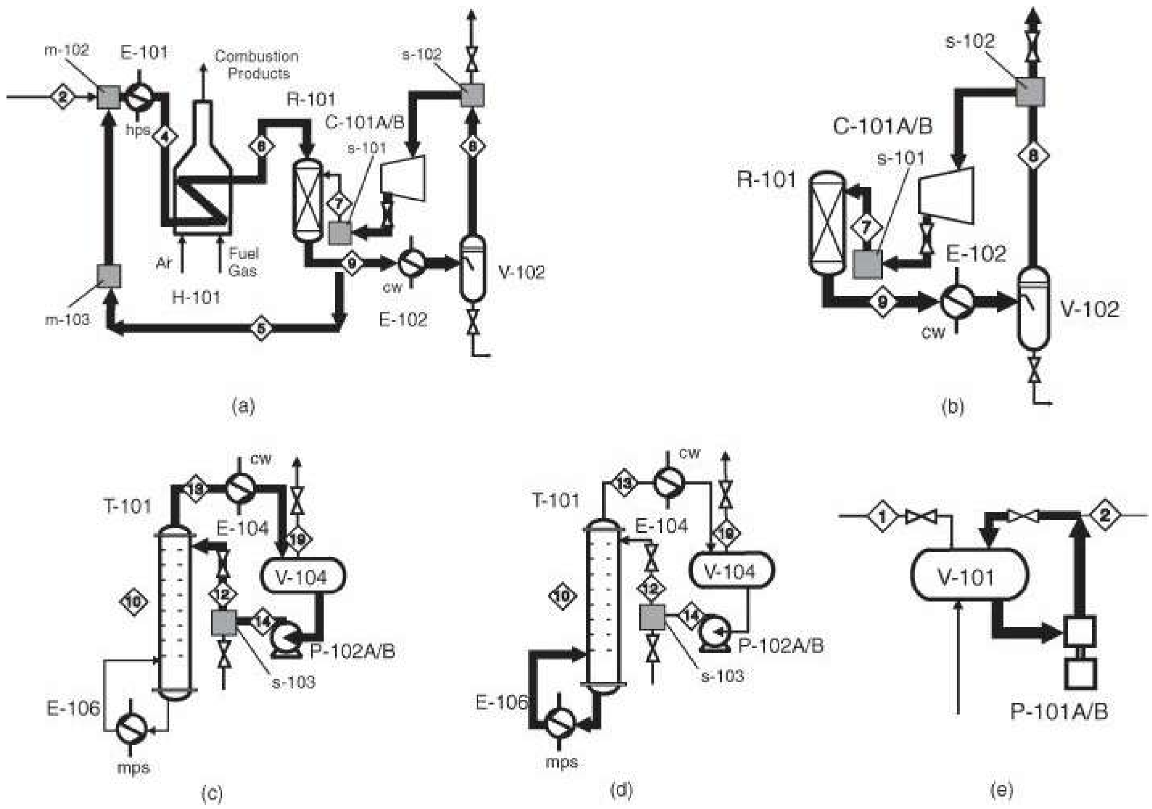

Figure E5.3(b). Identification of Other Recycle Loops in Toluene Hydrodealkylation PFD

This recycle loop is used for control purposes (see Chapter 18) and is not discussed further here. The logic used to deduce what chemical is being recycled in each loop is discussed in the next example.

The bypass streams are identified in Figure E5.3(c). These bypass streams contain mostly hydrogen and methane and are combined to form the fuel gas stream, Stream 16.

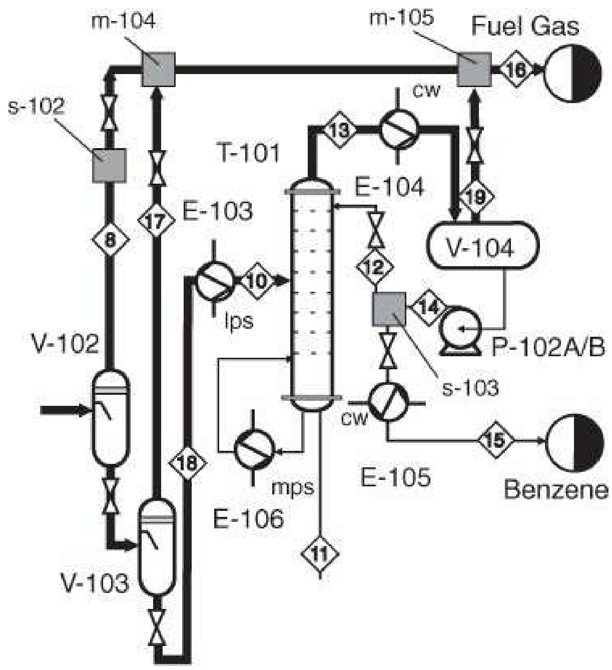

Figure E5.3(c). Identification of Bypass Streams in Toluene Hydrodealkylation PFD

It is important to remember that flow diagrams represent the most meaningful and useful documents to describe and understand a process. Although PFDs contain a lot of process information, it is sometimes necessary to apply additional knowledge about a unit operation to determine which chemicals are contained in a recycle stream. This idea is demonstrated in Example 5.4.

Example 5.4.

Provide preliminary identification of the important chemical species in each of the three recycle streams identified in Example 5.3. See Figures E5.3(a), E5.3(b)(a), and E5.3(b)(b).

Figure E5.3(a)

Stream 11: This is the bottoms product stream out of the distillation tower that provides the product benzene as distillate. The bottoms product stream must have a lower volatility than benzene. The only possible candidate is toluene. Stream 11 is essentially all toluene.

Figures E5.3(b)(a) and E5.3(b)(b)

Two undesignated streams leave splitter s-102: One stream leaves as part of a product stream and joins with other streams to form Stream 16. The other stream passes through C-101 to splitter s-101. The input and the two streams leaving s-101 have the same composition. If any of the stream compositions are known, then they are all known. In addition, methane is a reaction product and must leave the process. There are only two streams that leave the process, namely, Streams 15 and 16. Because the methane is unlikely to be part of the benzene stream, it must therefore be in the stream identified as fuel gas, Stream 16. The assumption is made that the product stream leaving is gaseous and not pure methane. If it were pure, it would be labeled methane.

The only other gas that could be present is hydrogen. Therefore, the fuel gas stream is a mixture of methane and hydrogen, and all three streams associated with s-101 have the same composition of methane and hydrogen.

The stream that leaves splitter s-102 and goes through compressor C-101 to splitter s-101 is split further into Streams 5 and 7. All streams have the same composition.

Stream 5 then mixes with additional hydrogen from Stream 3 in mixer m-103. The stream leaving m-103 contains both hydrogen and methane, but with a composition of hydrogen greater than that in the other gas streams discussed.

Finally, Stream 7, which also leaves splitter s-101, flows back to the reactor and forms the third recycle stream.

Before the analysis in Example 5.4 can be accepted, it is necessary to check out the assumption used to develop the analysis. Up to this point, the skeleton flow diagram was used, but it did not provide the important temperatures, pressures, and flowrates that are seen in the completed PFD (Figure 1.5). Figure 1.5 gives the following information for the flowrates of reactants:

Hydrogen (Stream 3): 572 kg/h (286.0 kmol/h)
Toluene (Stream 1): 10,000 kg/h (108.7 kmol/h)

Based on the information given in Table 1.5, only 108 kmol/h of hydrogen reacts to form benzene, and 178 kmol/h is excess reactant that leaves in the fuel gas. The fuel gas content is about 40 mol% methane and 60 mol% hydrogen. This confirms the assumption made in Example 5.4.

5.4. Tracing Nonreacting Chemicals

Chemical processes often contain nonreacting, or inert, compounds. These chemicals must appear in both the input and output streams and are neither created nor destroyed in the process. Unlike the reactants, it makes no difference in what direction these nonreacting chemicals are traced. They can be traced in the forward direction, the backward direction, or, starting in the middle, they can be traced in both directions. Other than this additional flexibility, the tactics provided above can be applied to all nonreacting chemicals.

5.5. Limitations

When the tracing procedure resorts to combining several unit operations into a single system that provides a single stream, the path is incomplete. This can be seen in the paths of both product streams, methane and benzene, in Figure E5.1.

> **Benzene:** The benzene flows into and out of the distillation system as the figure shows. There is no indication how it moves through the internal units consisting of V-104, s-103, E-104, E-106, and T-101.
>
> **Methane:** The methane flows into and out of a system composed of V-102, V-103, s-102, and m-104. Again, there is no indication of the methane path.

In order to determine the performance and the flows through these compound systems, you need more information than provided in the skeleton PFD, and you must know the function of each of the units.

The development given in the previous sections used only the information provided on the skeleton PFD, without the description of the unit operation, and did not include the important flows, temperatures, and pressures that were given in the full PFD (Figure 1.5) and the flow table (Table 1.5). With this additional information and knowledge of the unit operations, you will be able to fill in some of the paths that are yet unknown.

Each step in tracing the flow paths increases our understanding of the process for the production of benzene represented in the PFD. As a last resort, reference should be made to the flow table to determine the composition of the streams, but this fails to develop analytical skills that are essential to understand the process.

5.6. Written Process Description

A process description, like a flow table, is often included with a PFD. When a description is not included, it is necessary to provide a description based upon the PFD. Based on the techniques developed in this and Chapter 1, you should be able to write a detailed description of the toluene hydrodealkylation process. Table 5.1 provides such a description. You should read this description carefully and make sure you understand it fully. It would be useful, if not essential, to refer to the PFD in Figure 1.5 during your review. It is a good idea to have the PFD in front of you while you follow the process description.

Table 5.1. Process Description of the Toluene Hydrodealkylation Process (Refer to Figures 5.3 and 1.5)

Fresh toluene, Stream 1, is combined with recycled toluene, Stream 11, in the storage tank, V-101. Toluene from the storage tank is pumped, via P-101, up to a pressure of 25.8 bar and combined with the recycled and fresh hydrogen streams, Streams 3 and 5. This two-phase mixture is then fed through the feed preheater exchanger, E-101, where its temperature is raised to 225°C, and the toluene is completely vaporized. Further heating is accomplished in the heater, H-101, where the temperature of the stream is raised to 600°C. The stream leaving the heater, Stream 6, enters the reactor, R-101, at 600°C and 25.0 bar. The reactor consists of a vertical packed bed of catalyst, down through which the hot gas stream flows. The hydrogen and toluene react catalytically to produce benzene and methane according to the following exothermic reaction:

$$\underset{\text{toluene}}{C_7H_8} + H_2 \rightarrow \underset{\text{benzene}}{C_6H_6} + CH_4$$

The reactor effluent, Stream 9, consisting of benzene and methane produced from the reaction, along with the unreacted toluene and hydrogen, is quenched in exchanger E-102, where the temperature is reduced to 38°C using cooling water. Most of the benzene and toluene condenses in E-102, and the two-phase mixture leaving this exchanger is then fed to the high-pressure phase separator, V-102, where the liquid and vapor streams are allowed to disengage.

The liquid stream leaving V-102 is flashed to a pressure of 2.8 bar and is then fed to the low-pressure phase separator, V-103. The liquid leaving V-103, Stream 18, contains toluene and benzene with only trace amounts of dissolved methane and hydrogen. This stream is heated in exchanger E-103 to a temperature of 90°C prior to being fed to the benzene purification column, T-101. The benzene column, T-101, contains 42 sieve trays and operates at approximately 2.5 bar. The overhead vapor, Stream 13, from the column is condensed using cooling water in E-104, and the condensate is collected in the reflux drum, V-104. Any methane and hydrogen in the column feed accumulates in V-104, and these noncon-densables, Stream 19, are sent to fuel gas. The condensed overhead vapor stream is fed from V-104 to the reflux pump P-102. The liquid stream leaving P-102, Stream 14, is split into two, one portion of which, Stream 12, is returned to the column to provide reflux. The other portion of the condensed liquid is cooled to 38°C in E-105, prior to being sent to storage as benzene product, Stream 15. The bottoms product from T-101, Stream 11, contains virtually all of the toluene fed to the column and is recycled back to V-101 for further processing.

The vapor stream leaving V-102 contains most of the methane and hydrogen in the reactor effluent stream plus small quantities of benzene and toluene. This stream is split into two, with one portion being fed to the recycle gas compressor, C-101. The stream leaving C-101 is again split into two. The major portion is contained in Stream 5, which is recycled back to the front end of the process, where it is combined with fresh hydrogen feed, Stream 3, prior to being mixed with the toluene feed upstream of E-101. The remaining gas leaving C-101, Stream 7, is used for temperature control in the reactor, R-101. The second portion of the vapor leaving V-102 constitutes the major portion of the fuel gas stream. This stream is first reduced in pressure and then combined with the flashed vapor from V-103, Stream 17, and with the noncondensables from the overhead reflux drum, Stream 19. The combination of these three streams is the total fuel gas product from the process, Stream 16.

The process description should capture all the knowledge that you have developed in the last two chapters and represents a culmination of our understanding of the process up to this point.

5.7. Summary

This chapter showed how to trace many of the chemical species through a PFD, based solely upon the information shown on the skeleton PFD. It introduced operations involving splitting and mixing, not explicitly shown on the PFD, which were helpful in tracing these streams.

For situations where there was no single input or output stream, systems containing multiple unit operations were created. The tracing techniques for these compound systems did not provide the information needed to determine the internal flows for these systems. In order to determine reflux ratios for columns, for example, the process flow table must be consulted.

With the information provided, an authoritative description of the process can be prepared.

What You Should Have Learned

- Each component within a continuous chemical process can be traced.
- The tracing of chemical components is achieved using simple rules.

Problems

Identify the main reactant and product process streams for the following:

1. The ethylbenzene process shown in Figure B.2.1, Appendix B
2. The styrene production facility shown in Figure B.3.1, Appendix B
3. The drying oil production facility shown in Figure B.4.1, Appendix B
4. The maleic anhydride production process shown in Figure B.5.1, Appendix B
5. The ethylene oxide anhydride production process shown in Figure B.6.1, Appendix B
6. The formalin production process shown in Figure B.7.1, Appendix B

Identify the main recycle and bypass streams for the following:

7. The styrene production facility shown in Figure B.3.1, Appendix B
8. The drying oil production facility shown in Figure B.4.1, Appendix B
9. The maleic anhydride production process shown in Figure B.5.1, Appendix B

Write a process description for the following:

10. The ethylbenzene process shown in Figure B.2.1, Appendix B
11. The drying oil production facility shown in Figure B.4.1, Appendix B
12. The ethylene oxide production facility shown in Figure B.6.1, Appendix B