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Material Balance Calculation for Processes with Recycle Streams Using the Initial Zero Recycle Method

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Abstract: A method called the initial zero recycle method has been proposed for the calculation of the material balance of processes with recycle streams. The method is a modification of the classical Cut And Try Method. The proposed method has been illustrated with the calculation of the material balance of the industrial process for the synthesis of cumene (isopropylbenzene) from benzene and propylene at 623 K (350°C) and 30 atm. The results show that the solution of the material balance of the process was achieved at the end of four iteration cycles.

Key words: Material balance calculation, streams with recycle, cut and try method, modified cut and try method, initial zero recycle method

INTRODUCTION

A complete material balance is the single most important component of a chemical engineering process design. It determines the process stream flow rates and their compositions, the sizes of the various items of equipment, the energy balance of the process and the heat duties of heat transfer equipment. A material balance is required in the simulation and optimization of processes, in trouble-shooting, in the location of material loss, in the comparison of plant performance data against design data, in the extrapolation of data obtained from plant instrumentation and in the monitoring and control of instrument performance.

In mass balance calculations, the presence of recycle streams makes the calculations more difficult. The more recycle streams there are, the more complex and difficult the material balance calculations become. If no recycle streams are present, the material balance calculation on a series of processing steps is straightforward and can be carried out sequentially, taking each processing step one after the other. The calculated flow rates out of one processing step become the feed flow rates to the next step. If a recycle stream is present, then at the point where the recycle stream is returned to the process, the flow rate of the recycle stream is unknown, as its value depends on downstream flow rates which have not yet been calculated. Since the recycle flow rate is unknown, the sequence of calculations cannot be continued to the point where the flow rate of the recycle stream can be determined.

There are 2 traditional methods of solution of the material balance of processes with recycle streams, viz. The Cut and Try Method and The Formal Algebraic Method (Sinnott, 1999).

The cut and try method: In this method, the recycle stream flow rates are estimated and the calculations are continued until the recycle flow rates are calculated. The estimated flow rates are then compared with the calculated value and a better estimate of the recycle flow rate is made. The procedure is continued until the difference between the estimated and the calculated flow rates is within a desired tolerance. This method is known by other names: Tearing method (Henley and Rosen, 1969; Reklaitis and Schneider, 1983), sequential modular method (Sinnott, 1999), sequential modular strategy (Reklaitis and Schneider, 1983). Strategies can be deviced to force the iteration procedure to converge more rapidly, for example, the convergence block concept of Henley and Rosen (1969).

The formal algebraic method: In this method, it is realized that the presence of recycle streams implies that some of the mass balance equations have to be solved simultaneously. The simultaneous equations are set up with the recycle flow rates as unknowns and are solved using the standard methods for solving simultaneous equations. This method is also known as the equation based method (Sinnott, 1999).

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The cut and try method: Appears to be simpler to apply than the Formal Algebraic Method and requires only moderate computing power when computer solution is employed. However, computational difficulties may arise with this method as a result of the iterative methods used to solve recycle problems and attain convergence. A major limitation of the Cut and Try Method is its inability to simulate the dynamic, time dependent, behaviour of processes, since it is a steady-state simulation method. Nevertheless, the method has considerable physical appeal in that the iterations can be assumed to approximate the transient start-up of a real plant. Hopefully, just as the real plant comes to steady state so will the iterations in this method eventually converge. If difficulty in convergence is experienced, this may mean that the real plant may have difficulties in achieving steady state during start-up or in recovering from an upset.

The formal algebraic method: The formal algebraic method can simulate the unsteady state operation of processes and equipment as the entire process can be described by a set of simultaneous differential equations, which can be solved simultaneously not stepwise as in The Cut and Try Method. Dynamic simulators based on the Formal Algebraic Method require more computer power than steady-state simulators. This is because of the need to solve the many differential equations which are needed to describe a process or even a single item of equipment. However, since fast, powerful computers are now available, this is no longer a constraint. By its nature, The Formal Algebraic Method does not suffer from the problems of recycle convergence inherent in The Cut and Try Method. Since temperature, pressure and flow rate are not fixed and the input of one unit is not determined by the calculated output from the previous unit in the sequence, as is the case with steady-state simulators, The Formal Algebraic Method demands more computer time than The Cut and Try Method. The main advantage of the Formal Algebraic Method is its ability to model the unsteady-sate, transient conditions that occur in the system. For this reason, this method is increasingly being used in safety studies and control systems design.

The theory of recycle processes published by Nagiev (1964) is a Formal Algebraic Method and uses the concept of split-fractions to set up the set of simult-aneous equations which describe the mass balance of a process. Nagiev (1964) theory has been employed by Rosen (1962), Henley and Rosen (1969), Sinnott (1999) and Onyelucheya (2008) to solve the mass balance of chemical processes.

Some proprietary computer software packages which make use of the above methods to solve the material balances of recycle processes have been developed for use in chemical process simulation. They include the following: HYSYS, ASPEN-10, MASSBAL CHEM-CAD, DESIGN II, FLOWTRAN, PRO/II, UNIOPT, FLOWPACK, SPEEDUP, AS-EASY-AS, CHESS, CHEOPS, UWOPS, CHIPS, FLEXIFLOW, POWERFACTS, PACER, CHEVRON, PROVISION, EASYBAL. Further information on these programs can be obtained from the World Wide Web and from the conventional literature, Sinnott (1999), Onyelucheya (2008).

THE INITIAL ZERO RECYCLE METHOD

A modification of the Cut and Try Method described above and in Sinnott (1999) is hereby proposed. It has been named, The Initial Zero Recycle Method. The classical Cut and Try Method is identical with the Tearing and the Convergence Block Concept described by Henley and Rosen (1969). In both methods, each recycle stream is regarded as a tear stream. By tearing, the stream is meant that the value of the tear stream, is estimated and that the calculation of the material balance of a process then proceeds. Since, the value of the tear stream was originally estimated, the new value may not be the same as the estimated value. Hence, the new calculated value of the tear stream is given a new name and a convergence block is inserted into the place where the recycle stream was torn. Consider, for example, the process shown in Fig. 1. Although, stream S1 is known, block A1 cannot be calculated, since stream S4 is unknown. So stream S4 is torn, stream S4 is estimated and streams S2, S3, S4 and S5 are calculated in sequence by calculating units A1, A2 and A3. Since S4, was originally estimated, the calculated stream S4 may not be the same as the estimated S4; hence, the calculated stream S4 is relabeled as S6 and a convergence block A4 is inserted into the place where stream S4 was torn, as is shown in Fig. 2.

The advantage of inserting the convergence block is that it can be treated like any other building block. The function of the convergence block is to force stream S4 (the output stream from the convergence block) to be equal to S6 (the input stream). The order in which the building blocks can be solved is shown in Fig. 3, after estimating block A4.

We now compare stream S6 with stream S4. If convergence is achieved, the calculation is completed. If not, S4 is re-estimated and another calculation cycle is commenced.

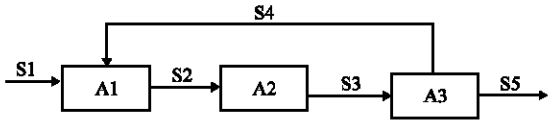


Fig. 1: A process with one recycle stream

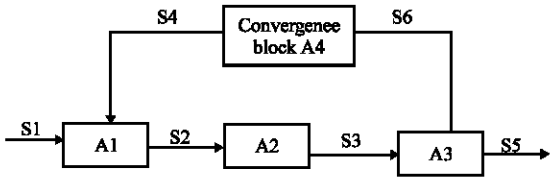


Fig. 2: Insertion of a convergence block in the recycle stream

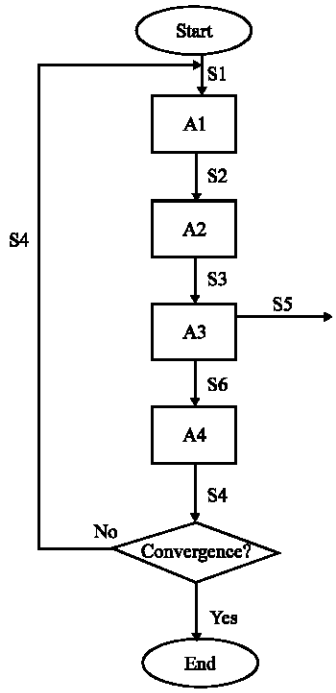


Fig. 3: Block diagram of order of calculation

Tearing of complex processes may become difficult as it may not be obvious, which streams should be torn. Generally, a tear stream is selected and the calculation is continued until it comes back to the torn stream. The convergence block is then inserted at that point. If a path cannot be found back without estimating other streams, another tear point is tried. Sometimes, it is necessary to tear two or more streams simultaneously. Generally, effort is made to minimize the number of streams to tear, but this may not always be the best strategy.

Sometimes, more than one recycle stream must be torn and the convergence of the streams must be forced simultaneously. The torn streams are estimated and become the starting point of the calculation.

The modified cut and try method: Proposed here for solving the complete material balance of a complex process involving any number of recycle streams is a modification of the classical Cut and Try Method described above and in the literature, Sinnott (1999) and Henley and Rosen (1969): At the beginning of the first iteration cycle through the process, the recycle streams are assumed to have no flow values. Therefore, the values of the component flows and other properties of these streams are set equal to zero for the first iteration cycle. The values of these properties of the recycle streams at the end of the first iteration cycle are used as the starting properties at the beginning of the second iteration cycle. This procedure is repeated until the properties of all the streams of the process remain constant or until the properties of a particular stream differ from the values obtained in the previous cycle for the same stream by a small value, criterion or tolerance which can be arbitrarily set. The iteration is then assumed to have converged.

As is the case with the classical Cut and Try Method, the advantage of this proposed method is that it is ideally suited to be programmed on the computer so that the iterative procedure involved, no matter how complex and tedious, can be completed rapidly. It may be faster than the tearing and the convergence block concept method, Henly and Rosen (1969). Another advantage is that as was stated above, the method has considerable physical appeal in that the iterations can be stated in such a way that they approximate the transient start -up behaviour of a real plant. Just as a real plant eventually attains steady state after start-up so may the iterations converge. If difficulty in convergence is experienced, the real plant may have difficulty in start-up or in recovering after an upset.

THE PROCEDURE OF THE INITIAL ZERO RECYCLE METHOD

The complete material balance is solved by iteration in cycles. The procedure for carrying out the calculations is the following.

The first cycle of the iteration procedure is initiated by moving in a sequential modular manner from unit to unit until the calculations of the last unit have been completed. For the first cycle the variables of the recycle streams are set equal to zero. It is convenient to initiate the calculation at the feed stream end or at the product

stream end of the process, depending on the end where most information on the process is available. For example, if the quantity of feed to be processed is given as well as other data regarding the feed, the calculation could be commenced at the feed stream end. If the quantity of product to be produced is given as well as other data regarding the product stream, the calculation could be initiated at the product end.

Subsequent cycles are calculated in a similar manner. The result of the recycle streams at the end of a cycle is used directly to calculate the next cycle. The procedure is continued until the iteration converges that is, until the properties of a particular stream differ from the values obtained in the previous cycle by a small value which can be arbitrarily set.

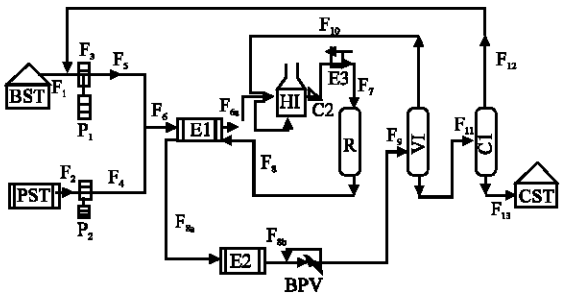
ILLUSTRATION OF THE INITIAL ZERO RECYCLE METHOD

Process description: The process used to illustrate the proposed method is the synthesis of cumene (isopropylbenzene) from benzene and propylene, shown as a process flow diagram in Fig. 4. The reaction is given by the following stoichiometric equation:

$$C_6H_{6(g)} + C_3H_{6(g)} \rightleftharpoons C_9H_{12(g)}$$

In this process, cumene is produced by passing a gaseous mixture of benzene and propylene over a suitable catalyst in a tubular reactor, R. The reactants are pumped from storage tanks, are mixed and are allowed to exchange heat with the reactor effluent stream in a heat exchanger. E1, are vaporized in a furnace H1, are compressed to the reaction pressure of 30 at in a compressor C3, are adjusted to the reaction temperature of 623 K (350°C) in a heat exchanger E3 and are fed to the reactor. The product gases exchange heat with the reactor inlet stream in the heat exchanger E1. The product gases are further cooled in another heat exchange E2 to condense essentially all the cumene and unreacted benzene in the product stream. The unreacted propylene in the product stream is completely separated from the liquid component of the reactor effluent stream in a low pressure separator V1 which is maintained at 1atm pressure and 623 K (350°C). The propylene is used to fire the furnace.

The liquid stream from the separator is fed to a distillation column, C1, which separates the benzene from the cumene. The cumene product stream leaves at the bottom of the column, while the benzene stream leaves at the top and is recycled to the fresh benzene feed stream.



Process equipment

BST = Benzene storage tank

PST = Propylene storage tank

P_1 = Benzene pump

P_2 = Propylene pump

E1 = Reactor effluent heat exchanger

H1 = Furnace

R = Fixed bed catalytic reactor

E2 = Flash vessel heat exchanger

V1 = Flash vessel

C1 = Distillation Column

BPV = Back pressure valve

C2 = Compressor

E3 = Heat exchanger

CST = Cumene storage tank

Process streams

F_1 = Pure benzene feed

F_2 = Pure propylene feed

F_3 = Benzene make up (F_1) + Benzene recycle (F_{12})

F_4 = Propylene pump exit stream

F_5 = Benzene pump exit stream

F_6 = Benzene stream (F_5) + propylene stream (F_4)

F_{6a} = Heat exchanger (EI) outlet stream

F_7 = Reactor inlet stream

F_8 = Reactor outlet stream

F_{8a} =Heat exchanger outlet stream

F_{8b} =Back pressure valve inlet stream

F_9 = Flash vessel inlet stream

F_{10} = Flash vessel outlet stream

F_{11} = Flash vessel outlet vapour stream

F_{12} = Distillation column liquid stream

F_{13} = Distillation column bottom stream

Fig. 4: The manufacture of cumene

Design data: The following design data apply:

- Quantity of cumene in the cumene product stream is 100,000 metric tons/stream year
- Basis of calculation is 8000 h/stream year
- Reactor temperature is 623 K (350°C)
- Reactor pressure is 30 atm
- The molar ratio of benzene to propylene in the reactor inlet stream is 2:1
- The conversion of propylene in the reactor is 99%
- The product cumene purity level is 99 wt%, the balance being benzene
- The recycle benzene purity is 90 wt%, the balance being cumene
- The cumene going into the distillation column that leaves in the cumene product stream is 90 wt%
- Assume that all vapours are ideal gases and that all liquid mixtures are ideal solutions

The block diagram for the calculations, using the procedure described above is displayed in Fig. 5.

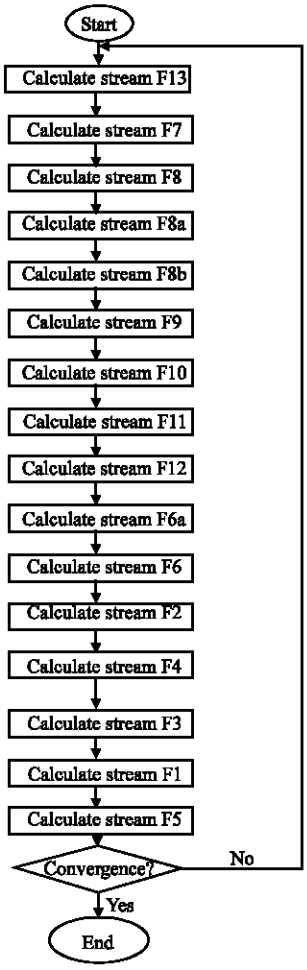


Fig. 5. The block diagram of the calculations

RESULTS AND DISCUSSION

The complete material balance was solved manually following the procedure described above and shown as a block diagram in Fig. 5. The results show that the iteration converged after 4 cycles. The material balance at the end of each of the 4 cycles is shown in Table 1. The material balance at the end of the 4rth cycle is taken to be the authentic material balance of the process.

The results shown in Table 1 clearly indicate that there is no significant difference between the compositions of the various streams at the ends of the 3rd and 4rth cycles of the iterative calculation. This is interpreted to mean that the iterative sequential modular material balance calculation has converged after the 4th cycle. The flow rates of the streams at the end of the 4th cycle are taken as the authentic material balance of the process.

Table 1: Summary of the material balance calculations

Stream	Component (gmol s^{-1})	Cycle 1	2	3	4
1	Benzene	64.94	26.11	29.39	29.39
	Propylene	-	-	-	-
	Cumene	-	-	-	-
2	Benzene	-	29.23	-	-
	Propylene	32.47	-	29.23	29.23
	Cumene	-	-	-	-
3	Benzene	64.94	58.45	58.45	58.45
	Propylene	-	-	-	-
	Cumene	-	3.21	3.21	3.21
4	Benzene	-	-	-	-
	Propylene	32.47	29.23	29.23	29.23
	Cumene	-	-	-	-
5	Benzene	64.94	58.45	58.45	58.45
	Propylene	-	-	-	-
	Cumene	-	3.21	3.21	3.21
6	Benzene	64.94	58.45	58.45	58.45
	Propylene	32.47	29.23	29.23	29.23
	Cumene	-	3.21	3.21	3.21
6a	Benzene	64.94	58.45	58.45	58.45
	Propylene	32.47	29.23	29.23	29.23
	Cumene	-	3.21	3.21	3.21
7	Benzene	64.94	58.45	58.45	58.45
	Propylene	32.47	29.23	29.23	29.23
	Cumene	-	3.21	3.21	3.21
8	Benzene	32.79	29.51	29.51	29.51
	Propylene	0.32	0.29	0.29	0.29
	Cumene	32.15	32.15	32.15	32.15
8a	Benzene	32.79	29.51	29.51	29.51
	Propylene	0.32	0.29	0.29	0.29
	Cumene	32.15	32.15	32.15	32.15
8b	Benzene	32.79	29.51	29.51	29.51
	Propylene	0.32	0.29	0.29	0.29
	Cumene	32.15	32.15	32.15	32.15
9	Benzene	32.79	29.51	29.51	29.51
	Propylene	0.32	0.29	0.29	0.29
	Cumene	32.15	32.15	32.15	32.15
10	Benzene	-	-	-	-
	Propylene	0.32	0.29	0.29	0.29
	Cumene	-	-	-	-
11	Benzene	32.34	29.51	29.61	29.61
	Propylene	-	-	-	-
	Cumene	3.21	32.15	32.15	32.15
12	Benzene	32.34	29.06	29.06	29.06
	Propylene	-	-	-	-
	Cumene	3.21	3.21	3.21	3.21
13	Benzene	0.45	0.45	0.45	0.45
	Propylene	-	-	-	-
	Cumene	28.94	28.94	28.94	28.94

The manual calculations involved in this simple iterative procedure show that for larger and more complex problems involving more recycle streams, the calculations would consume many man-days of calculation. The repetitive, iterative nature of the calculations is clear evidence that computer-aided calculation is indicated.

CONCLUSION

A method for the calculation of the material balance of processes with recycle streams has been proposed. The method is a modification of the classical Cut and Try

Method. The proposed method has been used to calculate the material balance of the industrial process for the synthesis of cumene (isopropylbenzene) from benzene and propylene at 623 K (350°C) and 30 atm. The results show that the solution of the material balance of the process was achieved in 4 iteration cycles.

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