

## Computer-Aided Material Balance Calculation of Processes with Recycle Streams using the Initial Zero Recycle Method

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**Abstract:** A computer-aided method for the calculation of the material balance of processes with recycle streams has been shown. The procedure used for the material balance calculation is the Initial Zero Recycle Method. The process used to describe the method is the industrial synthesis of cumene (isopropylbenzene) from benzene and propylene at 623 K (350°C) and 30 ATM. The results show that the iterative solution of the material balance of the process converged in four iteration cycles.

**Key words:** Computer-aided material balance, recycle streams, Initial Zero Recycle Method, iterative solution, industrial synthesis, Nigeria

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### INTRODUCTION

There are two traditional methods of solving the material balance of processes with recycle streams, viz., the Cut and Try Method and the Formal Algebraic Method (Sinnott, 1999; Aneke and Oyoh, 2008). The Cut and Try 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).

A method called The Initial Zero Recycle Method has recently been described for the same system (Aneke and Oyoh, 2008 and Aneke, 2009). The method is a modification of the classical Cut and Try Method (Sinnott, 1999) which is identical with the Tearing and the Convergence Block Concept described by Henley and Rosen (1969).

In both the classical Cut and Try Method and the Initial Zero Recycle Method, each recycle stream is regarded as a tear stream (Henley and Rosen, 1969; Aneke and Oyoh, 2008).

As the case with the classical Cut and Try Method, the advantage of the Initial Zero Recycle Method is that it is ideally suited to be programmed on the computer so that the iterative procedure involved can be completed rapidly. Another advantage is that the method has

considerable physical appeal in that the iterations involved can be stated in such a way that they approximate the transient start-up behaviour of an actual process plant. In the same way that a real plant eventually attains steady state after start-up, so may the iterations eventually converge. If difficulty in convergence is experienced, this may mean that the real plant may experience difficulty in start-up or in recovering after an upset.

The Initial Zero Recycle Method has been described with the manual calculation of the material balance of the industrial synthesis of cumene (isopropylbenzene) from benzene and propylene at 623 K (350°C) and 30 atm (Aneke and Oyoh, 2008; Aneke, 2009). The results showed that the manual solution of the material balance of the process was achieved in 4 iteration cycles.

### MATERIALS AND METHODS

**The procedure of the computer-aided application 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 from one end of the process to the other until the calculations of the last unit have been completed. For the first cycle the variables of the recycle streams are set equal to 0. 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 shown 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 shown 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 for the same stream by a small value which can be arbitrarily set

**Process equipment:** BST = Benzene Storage Tank, PST = Propylene Storage Tank, P<sub>1</sub> = Benzene pump, P<sub>2</sub> = Propylene pump, E<sub>1</sub> = Reactor effluent heat exchanger, H<sub>1</sub> = Furnace, R = Fixed bed catalytic reactor, E<sub>2</sub> = Flash vessel heat exchanger, V<sub>1</sub> = Flash vessel, C<sub>1</sub> = Distillation Column, BPV = Back pressure valve, C<sub>2</sub> = Compressor, E<sub>3</sub> = Heat exchanger, CST = Cumene Storage Tank.

**Process streams:** F<sub>1</sub> = Pure benzene feed, F<sub>2</sub> = Pure propylene feed, F<sub>3</sub> = Benzene make up (F<sub>1</sub>) + Benzene recycle (F<sub>12</sub>), F<sub>4</sub> = Propylene pump exit stream, F<sub>5</sub> = Benzene pump exit stream, F<sub>6</sub> = Benzene stream (F<sub>5</sub>) + propylene stream (F<sub>4</sub>), F<sub>6a</sub> = Heat exchanger (E<sub>1</sub>) outlet stream, F<sub>7</sub> = Reactor inlet stream, F<sub>8</sub> = Reactor outlet stream, F<sub>8a</sub> = Heat exchanger outlet stream, F<sub>8b</sub> = Back pressure valve inlet stream, F<sub>9</sub> = Flash vessel inlet stream, F<sub>10</sub> = Flash vessel outlet stream, F<sub>11</sub> = Flash vessel outlet vapour stream, F<sub>12</sub> = Distillation column liquid stream, F<sub>13</sub> = Distillation column bottom stream.

**Illustration of the computer-aided application of the Initial Zero Recycle Method**

**Process description:** The process used to describe the proposed method is the synthesis of cumene (isopropylbenzene) from benzene and propylene

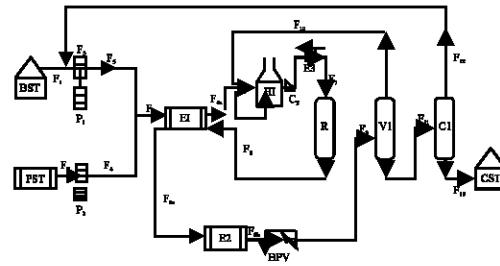
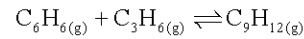


Fig. 1: The manufacturer of cumene

shown as a process flow diagram in Fig. 1. The reaction is shown by the following stoichiometric equation:



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.

E<sub>1</sub> are vaporized in a furnace H<sub>1</sub> are compressed to the reaction pressure of 30 atm in a compressor C<sub>2</sub> are adjusted to the reaction temperature of 623 K (350°C) in a heat exchanger E<sub>3</sub> and are fed to the reactor. The product gases exchange heat with the reactor inlet stream in the heat exchanger E<sub>1</sub>.

The product gases are further cooled in another heat exchange E<sub>2</sub> 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 V<sub>1</sub> which is maintained at 1 atm 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, C<sub>1</sub> 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.

**Design data:** The following design data apply:

- Quantity of cumene in the cumene product stream is 100,000 metric tons per stream year
- Basis of calculation is 8000 h per 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 computer solution:** The block diagram for the calculations using the procedure described earlier is displayed in Fig. 2.

The symbols used in the computer programme are explained in Appendix. The computer programme for the solution of the problem using the above design data was written in the Visual Basic Programming Language (Ike, 2007).

The procedure used in the computer solution is identical with the one used in the manual solution of the same problem which has been described elsewhere (Aneke and Oyoh, 2008). The complete computer programme is available (Ike, 2007).

**RESULTS AND DISCUSSION**

The complete material balance was solved using the computer programme and following the procedure described before and shown as a block diagram in Fig. 2.

The results show that as was the case with the manual solution of the same problem (Aneke and Oyoh, 2008), the iteration converged at the fourth cycle.

The material balance at the end of each of the four cycles is shown in Table 1-4. The material balance at the end of the 4th cycle. Table 4 is taken to be the authentic material balance of the process.

The results shown in Table 1-4 clearly indicate that there is no significant difference between the compositions of the various streams at the ends of the third and fourth cycles of the iterative calculation.

This is interpreted to mean that the iterative sequential modular material balance calculation has converged after the fourth cycle. The flow rates of the streams at the end of the 4th cycle as shown in Table 4 are taken as the authentic material balance of the process.

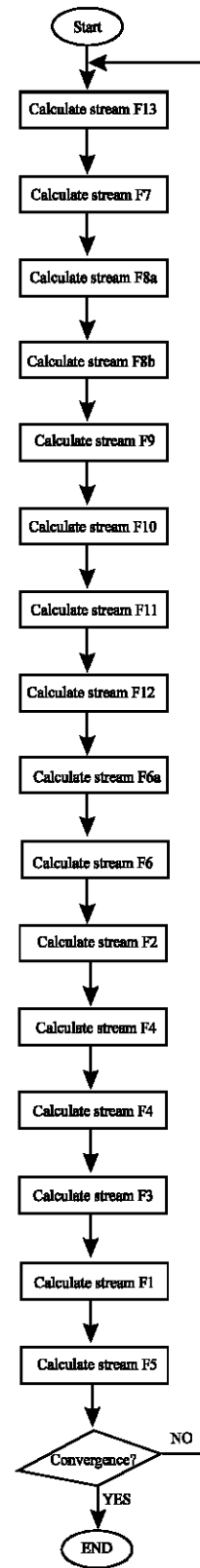


Fig. 2: The block diagram for the calculation



Table 4: Continued

P kg s <sup>-1</sup>	B kg s <sup>-1</sup>	C kg s <sup>-1</sup>	P kg mole s <sup>-1</sup>	B kg mole s <sup>-1</sup>	C kg mole s <sup>-1</sup>	Total kg s <sup>-1</sup>	Total kg mole s <sup>-1</sup>
1.229E+03	4.559E+03	3.858E+02	2.293E+01	5.845E+01	3.215E+00	6.174E+03	9.090E+01
1.229E+01	2.303E+03	3.858E+03	2.293E+01	2.952E+01	3.215E+01	6.173E+03	6.196E+01
1.229E+01	2.303E+03	3.858E+03	2.293E+01	2.952E+01	3.215E+01	6.173E+03	6.196E+01
1.229E+01	2.303E+03	3.858E+03	2.293E+01	2.952E+01	3.215E+01	6.173E+03	6.196E+01
1.229E+01	2.303E+03	3.858E+03	2.293E+01	2.952E+01	3.215E+01	6.173E+03	6.196E+01
1.229E+01	0.000E+00	0.000E+00	2.293E+01	0.000E+00	0.000E+00	1.229E+01	2.923E+01
0.000E+00	2.303E+03	3.858E+03	0.000E+00	2.952E+01	3.215E+01	6.161E+03	6.167E+01
0.000E+00	2.267E+03	3.858E+02	0.000E+00	2.907E+01	3.215E+00	2.653E+03	3.229E+01
0.000E+00	3.507E+01	3.472E+03	0.000E+00	4.497E+01	2.894E+01	3.507E+03	2.938E+01

P = Propylene; B = Benzene; C = Cumene

## APPENDIX

### Symbols used in the computer programme

F <sub>13</sub> CW = Weight of cumene in product, g/s	F <sub>13</sub> CM = Moles of cumene in product, g/s
F <sub>13</sub> BW = Weight of benzene in product, gmoles/s	F <sub>13</sub> BM = Moles of benzene in product, g/s
F <sub>13</sub> TW = Total weight of stream F <sub>13</sub>	F <sub>13</sub> TM = Total moles of stream F <sub>13</sub>
F <sub>11</sub> CW = Weight of cumene in stream F <sub>11</sub>	F <sub>11</sub> CM = Moles of cumene in stream F <sub>11</sub>
F <sub>11</sub> TW = Total weight of stream F <sub>11</sub>	F <sub>11</sub> TM = Total moles of stream F <sub>11</sub>
F <sub>11</sub> BW = Weight of benzene in stream <sub>11</sub>	F <sub>11</sub> BM = Moles of benzene in stream <sub>11</sub>
F <sub>11</sub> PW = Weight of propylene in stream <sub>11</sub>	F <sub>11</sub> PM = Moles of propylene in stream <sub>11</sub>
F <sub>8</sub> PM = Weight of benzene in stream <sub>8</sub>	F <sub>8</sub> BW = Moles of benzene in stream <sub>8</sub>
F <sub>8a</sub> BW = Weight of benzene in stream <sub>8a</sub>	F <sub>8a</sub> BM = Moles of benzene in stream <sub>8a</sub>
F <sub>8</sub> PW = Weight of propylene in stream <sub>8</sub>	F <sub>8</sub> PM = Moles of propylene in stream <sub>8</sub>
F <sub>8a</sub> PW = Weight of propylene in stream <sub>8a</sub>	F <sub>8a</sub> PM = Moles of propylene in stream <sub>8a</sub>
F <sub>8c</sub> W = Weight of cumene in stream <sub>8</sub>	F <sub>8</sub> CM = Moles of cumene in stream <sub>8</sub>
F <sub>8a</sub> CW = Weight of cumene in stream <sub>8a</sub>	F <sub>8a</sub> CM = Moles of cumene in stream <sub>8a</sub>
F <sub>8</sub> TW = Total weight of stream <sub>8</sub>	F <sub>8</sub> TM = Total moles of stream <sub>8</sub>
F <sub>8a</sub> TW = Total weight of stream <sub>8a</sub>	F <sub>8a</sub> TM = Total moles of stream <sub>8a</sub>
F <sub>8b</sub> PW = Weight of propylene in stream <sub>8b</sub>	F <sub>8b</sub> PM = Moles of propylene in stream <sub>8b</sub>
F <sub>8b</sub> BW = Weight of benzene in stream <sub>8b</sub>	F <sub>8b</sub> BM = Moles of benzene in stream <sub>8b</sub>
F <sub>8b</sub> CW = Weight of cumene in stream <sub>8b</sub>	F <sub>8b</sub> CM = Moles of cumene in stream <sub>8b</sub>
F <sub>8b</sub> TM = Total weight of stream <sub>8b</sub>	F <sub>8b</sub> TM = Total moles of stream <sub>8b</sub>
F <sub>9</sub> PM = Moles of propylene in stream F <sub>9</sub>	F <sub>9</sub> PM = Weight of propylene in stream F <sub>9</sub>
F <sub>9</sub> BM = Moles of benzene in stream F <sub>9</sub>	F <sub>9</sub> BM = Weight of benzene in stream F <sub>9</sub>
F <sub>9</sub> CW = Moles of cumene in stream F <sub>9</sub>	F <sub>9</sub> CM = Weight of cumene in stream F <sub>9</sub>
F <sub>9</sub> TM = Total weight of stream F <sub>9</sub>	F <sub>9</sub> TW = Total moles of stream F <sub>9</sub>
F <sub>10</sub> PM = Moles of propylene in stream F <sub>10</sub>	F <sub>10</sub> PM = Weight of propylene in stream F <sub>10</sub>
F <sub>10</sub> BM = Moles of benzene in stream F <sub>10</sub>	F <sub>10</sub> BM = Weight of benzene in stream F <sub>10</sub>
F <sub>10</sub> CW = Moles of cumene in stream F <sub>10</sub>	F <sub>10</sub> CM = Weight of cumene in stream F <sub>10</sub>
F <sub>10</sub> TM = Total mole of stream F <sub>10</sub>	F <sub>10</sub> TW = Total weight of stream F <sub>10</sub>
F <sub>7</sub> PM = Moles of propylene in stream F <sub>7</sub>	F <sub>7</sub> PM = Weight of propylene in stream F <sub>7</sub>
F <sub>7</sub> BM = Moles of benzene in stream F <sub>7</sub>	F <sub>7</sub> BM = Weight of benzene in stream F <sub>7</sub>
F <sub>7</sub> CW = Moles of cumene in stream F <sub>7</sub>	F <sub>7</sub> CM = Weight of cumene in stream F <sub>7</sub>
F <sub>7</sub> TM = Total moles of stream F <sub>7</sub>	F <sub>7</sub> TW = Total weight of stream F <sub>7</sub>
F <sub>6a</sub> PM = Moles of propylene in stream F <sub>6a</sub>	F <sub>6a</sub> PM = Weight of propylene in stream F <sub>6a</sub>
F <sub>6a</sub> BM = Moles of benzene in stream F <sub>6a</sub>	F <sub>6a</sub> BM = Weight of benzene in stream F <sub>6a</sub>
F <sub>6a</sub> CW = Moles of cumene in stream F <sub>6a</sub>	F <sub>6a</sub> CM = Weight of cumene in stream F <sub>6a</sub>
F <sub>6a</sub> TM = Total moles in stream F <sub>6a</sub>	F <sub>6a</sub> TW = Total weight in stream F <sub>6a</sub>
F <sub>6</sub> PM = Moles of propylene in stream F <sub>6</sub>	F <sub>6</sub> PM = Weight of propylene in stream F <sub>6</sub>
F <sub>6</sub> BM = Moles of benzene in stream F <sub>6</sub>	F <sub>6</sub> BM = Weight of benzene in stream F <sub>6</sub>
F <sub>6</sub> CW = Moles of cumene in stream F <sub>6</sub>	F <sub>6</sub> CM = Weight of cumene in stream F <sub>6</sub>
F <sub>6</sub> TM = Total moles in stream F <sub>6</sub>	F <sub>6</sub> TW = Total weight in stream F <sub>6</sub>

$F_5PM$	=	Moles of propylene in stream $F_5$	$F_5PM$	=	Weight of propylene in stream $F_5$
$F_5BM$	=	Moles of benzene in stream $F_5$	$F_5BM$	=	Weight of benzene in stream $F_5$
$F_5CW$	=	Moles of cumene in stream $F_5$	$F_5CM$	=	Weight of cumene in stream $F_5$
$F_5TM$	=	Total moles in stream $F_5$	$F_5TW$	=	Total weight in stream $F_5$
$F_3PM$	=	Moles of propylene in stream $F_3$	$F_3PM$	=	Weight of propylene in stream $F_3$
$F_3BM$	=	Moles of benzene in stream $F_3$	$F_3BM$	=	Weight of benzene in stream $F_3$
$F_3CW$	=	Moles of cumene in stream $F_3$	$F_3CM$	=	Weight of cumene in stream $F_3$
$F_3TM$	=	Total moles in stream $F_3$	$F_3TW$	=	Total weight in stream $F_3$
$F_4PM$	=	Moles of propylene in stream $F_4$	$F_4PM$	=	Weight of propylene in stream $F_4$
$F_{44}CW$	=	Moles of cumene in stream $F_4$	$F_4CM$	=	Weight of cumene in stream $F_4$
$F_4TM$	=	Total moles in stream $F_4$	$F_4TW$	=	Total weight in stream $F_4$
$F_2PM$	=	Moles of propylene in stream $F_2$	$F_2PM$	=	Weight of propylene in stream $F_2$
$F_2BM$	=	Moles of benzene in stream $F_2$	$F_2BM$	=	Weight of benzene in stream $F_2$
$F_2CW$	=	Moles of cumene in stream $F_2$	$F_2CM$	=	Weight of cumene in stream $F_2$
$F_2TM$	=	Total moles in stream $F_2$	$F_2TW$	=	Total weight in stream $F_2$
$F_1PM$	=	Moles of propylene in stream $F_1$	$F_1PM$	=	Weight of propylene in stream $F_1$
$F_1BM$	=	Moles of benzene in stream $F_1$	$F_1BM$	=	Weight of benzene in stream $F_1$
$F_1CW$	=	Moles of cumene in stream $F_1$	$F_1CM$	=	Weight of cumene in stream $F_1$
$F_1TM$	=	Total moles in stream $F_1$	$F_1TW$	=	Total weight in stream $F_1$

### CONCLUSION

A computer-aided method for the calculation of the material balance of processes with recycle streams has been shown. The method used is the Initial Zero Recycle Method. The process used to describe the method is the industrial synthesis of cumene (isopropylbenzene) from benzene and propylene at 623 K (350°C) and 30 atm. The computer programme was written in the Visual Basic Programming Language. The results show that the iterative solution of the material balance of the process converged in four iteration cycles.

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