

CHAPTER IV

SIMULATION RESULTS

The applications of the present program, which has been developed in the previous chapter, are shown in this chapter. To test the robustness of the present program, the existing steady state program, PRO II, is selected to calculate an initial steady state conditions to compare with the dynamic simulation program. After the acceptance of the present program, the application to a dynamic compartmental models by changing feed conditions, i.e., $\pm 15\%$ step changes, has been considered by comparing with the existing steady state program and the full-order model.

4.1 Examples of Application

The following two examples were selected to test the present program by comparing the results with the existing steady state program, PRO II. The first example problem taken from the design case of debutanizer of Bangchak Petroleum Industry Company Limited, was the full-order model with 6 components and 25 plate's column. The second example, the same as first example but using a compartmental technique, was five-compartmental model.

The instructions that follow illustrate how the program was run and what the outputs were obtained after a run. Three steps described in the previous chapter have been performed in each example. To distinguish the program statements from the user's responses, user-typed characters are underlined throughout these examples.

Example 1 : Dynamic distillationGiven : Table 4.1 shows the given data**Table 4.1 Data for Example 1.**

Characteristic of Column			Operating Condition					
Total number of plates (NT)	=	25	Pressure in top of column, psia (PB) = 126.57					
Number of trays in stripping section (NF)	=	9	Pressure in bottom of column, psia (PD) = 133.04					
Weir height in stripping section, inch (WHS)	=	3.44	Reboiler heat-duty, Btu/hr (QR) = 5,875,000					
Weir height in rectifying section, inch (WHR)	=	3.44	Reflux rate, lbmole/hr (R) = 1,000.00					
Column diameter in stripping section, inch (DS)	=	72.0	Vapour product, lbmole/hr (DV) = 0.00					
Column diameter in rectifying section, inch (DR)	=	72.0	Murphree vapor-phase efficiency = 0.90					
Weir length in stripping section, inch (WLS)	=	51.1						
Weir length in rectifying section, inch (WLR)	=	51.1						
Volumetric holdup in column base, ft ³ (MVB)	=	130.0						
Volumetric holdup in reflux drum, ft ³ (MVD)	=	7.87						
Feed Data								
Phase	Temp. (°F)	Feed Flowrate (lbmole/hr)	Propane X ₁	Isobutane X ₂	N-Butane X ₃	Isopentane X ₄	N-Pentane X ₅	N-Hexane X ₆
Liquid	233.60	1263.11	.38730E-1	.37720E-1	.16720	.20764	.22923	.31947
Vapour	233.60	1.90	.13531	.75961E-1	.27746	.19462	.18776	.12889

Source : Bangchak Petroleum Industry Company Limited.

Original result : Table 4.2 shows the original result calculated by the existing steady state program, PRO II.

Table 4.2 Original results for Example 1.

Tray	Temp. (°F)	Liquid Flowrate (lbmole/hr)	Propane X_1	Isobutane X_2	N-Butane X_3	Isopentane X_4	N-Pentane X_5	N-Hexane X_6
Bottoms	290.66	0.00	.30702E-5	.24437E-3	.47600E-2	.13585	.22011	.63904
1	277.52	2364.00	.11084E-4	.58146E-3	.98300E-2	.19153	.28323	.51482
2	268.88	2387.70	.35139E-4	.11800E-2	.17270E-1	.23231	.31737	.43184
3	263.12	2403.50	.10474E-3	.22100E-2	.27630E-1	.25764	.32858	.38387
4	258.80	2407.02	.30147E-3	.39100E-2	.41700E-1	.27040	.32563	.35806
5	254.66	2400.12	.84631E-3	.66600E-2	.60310E-1	.27347	.31461	.34411
6	249.98	2383.72	.23200E-2	.11000E-1	.83960E-1	.26832	.29861	.33578
7	244.04	2357.61	.61900E-2	.17510E-1	.11214	.25552	.27885	.32978
8	235.58	2318.68	.15910E-1	.26590E-1	.14209	.23520	.25568	.32452
9	223.52	2261.31	.38730E-1	.37720E-1	.16720	.20764	.22923	.31947
10	211.28	918.85	.41350E-1	.41970E-1	.19099	.28603	.27468	.16498
11	204.08	976.06	.43060E-1	.44880E-1	.20845	.34472	.28590	.72990E-1
12	200.12	1011.21	.44110E-1	.46840E-1	.22198	.38375	.27382	.29500E-1
13	197.42	1029.37	.44890E-1	.48520E-1	.23563	.40906	.25055	.11340E-1
14	195.08	1038.91	.45670E-1	.50440E-1	.25291	.42411	.22265	.42200E-2
15	192.56	1045.16	.46620E-1	.52980E-1	.27698	.42909	.19280	.15200E-2
16	189.32	1051.09	.47870E-1	.56520E-1	.31088	.42210	.16209	.53214E-3
17	185.18	1058.58	.49490E-1	.61440E-1	.35719	.40050	.13121	.17765E-3
18	180.14	1069.19	.51510E-1	.68040E-1	.41671	.36255	.10112	.56000E-4
19	174.56	1084.07	.53920E-1	.76500E-1	.48680	.30943	.73330E-1	.16444E-4
20	168.98	1103.20	.56720E-1	.86780E-1	.56034	.24661	.49550E-1	.44520E-5
21	163.76	1124.78	.60210E-1	.98770E-1	.62729	.18266	.31070E-1	.11078E-5
22	159.08	1145.69	.65750E-1	.11254	.67784	.12578	.18100E-1	.25452E-6
23	154.40	1162.67	.77530E-1	.12824	.70388	.80540E-1	.98100E-2	.54373E-7
24	148.46	1173.29	.10685	.14526	.69558	.47410E-1	.48900E-2	.10765E-7
25	137.84	1170.40	.18133	.15923	.63291	.24400E-1	.21300E-2	.18784E-8
Distillate	122.00	1000.00	.35394	.15614	.48014	.91300E-2	.65312E-3	.21086E-9

Source : Running data by existing steady state program, PRO II.

Program Execution :

Step 1 : Start-up procedure

Load the working program by typing the working file name.

A> DYNAMICS

Step 2 : Input data

Select the number from main menu to input data step by step. Input data to displayed questions. See underlined characters.

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 1



*** Component Selection ***

The name must be typed in CAPITAL LETTER

Total number of component (NC) = 6

Component Name no. 1 = PROPANE

Component Name no. 2 = ISOBUTANE

Component Name no. 3 = N-BUTANE

Component Name no. 4 = ISOPENTANE

Component Name no. 5 = N-PENTANE

Component Name no. 6 = N-HEXANE

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25
Number of trays in stripping section (NF) = 9
Weir height in stripping section (WHS) = 3.44
Weir height in rectifying section (WHR) = 3.44
Column diameter in stripping section (DS) = 72.0
Column diameter in rectifying section (DR) = 72.0
Weir length in stripping section (WLS) = 51.1
Weir length in rectifying section (WLR) = 51.1
Volumetric holdup in column base (MVB) = 130.0
Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : N

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 3

**** Operating Conditions ****

Pressure in top of column PD, (psia) = 126.57

Pressure in bottom of column PB, (psia) = 133.04

Reboiler heat-duty QR, (x 1,000 Btu/hr) = 4980.0

Reflux rate R, (moles/hr) = 1000.0

Vapor product from reflux drum DV, (moles/hr) = 0.0

Murphree vapor-phase tray efficiency EFF = 0.9

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 4

**** Feed Data ****

Liquid Feed flow rate (moles/hr) = 1263.11

Liquid Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.038730

ISOBUTANE = 0.037720

N-BUTANE = 0.16720

ISOPENTANE = 0.20764

N-PENTANE = 0.22923

N-HEXANE = 0.31947

**** Feed Data ****

Vapor Feed flow rate (moles/hr) = 1.9

Vapor Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.135310

ISOBUTANE = 0.075961

N-BUTANE = 0.277460

ISOPENTANE = 0.194620

N-PENTANE = 0.187760

N-HEXANE = 0.128890

Press ENTER to continue



**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results ∞

Please ENTER your selection : 5

**** Initial Conditions ****

Temperature in column base TB, (F) = 290.66

Composition in column base :

PROPANE	=	<u>0.30702E-5</u>
ISOBUTANE	=	<u>0.24437E-3</u>
N-BUTANE	=	<u>0.47600E-2</u>
ISOPENTANE	=	<u>0.13585</u>
N-PENTANE	=	<u>0.22011</u>
N-HEXANE	=	<u>0.63904</u>

**** Initial Conditions ****

Temperature in tray no. 1 (F) = 277.52

Liquid flow rate in tray no. 1 (moles/hr) = 2364.0

Composition in tray no. 1 :

PROPANE = 0.11084E-4

ISOBUTANE = 0.58146E-3

N-BUTANE = 0.98300E-2

ISOPENTANE = 0.19153

N-PENTANE = 0.28323

N-HEXANE = 0.51482

**** Initial Conditions ****

Temperature in tray no. 2 (F) = 268.88

Liquid flow rate in tray no. 2 (moles/hr) = 2387.7

Composition in tray no. 2 :

PROPANE = 0.35139E-4

ISOBUTANE = 0.11800E-2

N-BUTANE = 0.17270E-1

ISOPENTANE = 0.23231

N-PENTANE = 0.31737

N-HEXANE = 0.43184

**** Initial Conditions ****

Temperature in tray no. 3 (F) = 263.12

Liquid flow rate in tray no. 3 (moles/hr) = 2403.5

Composition in tray no. 3 :

PROPANE = 0.10474E-3

ISOBUTANE = 0.22100E-2

N-BUTANE = 0.27630E-1

ISOPENTANE = 0.25764

N-PENTANE = 0.32858

N-HEXANE = 0.38387

**** Initial Conditions ****

Temperature in tray no. 4 (F) = 258.80

Liquid flow rate in tray no. 4 (moles/hr) = 2407.02

Composition in tray no. 4 :

PROPANE = 0.30147E-3

ISOBUTANE = 0.39100E-2

N-BUTANE = 0.41700E-1

ISOPENTANE = 0.27040

N-PENTANE = 0.32563

N-HEXANE = 0.35806

**** Initial Conditions ****

Temperature in tray no. 5 (F) = 254.66

Liquid flow rate in tray no. 5 (moles/hr) = 2400.12

Composition in tray no. 5 :

PROPANE = 0.84631E-3

ISOBUTANE = 0.66600E-2

N-BUTANE = 0.60310E-1

ISOPENTANE = 0.27347

N-PENTANE = 0.31461

N-HEXANE = 0.34411

**** Initial Conditions ****

Temperature in tray no. 6 (F) = 249.98

Liquid flow rate in tray no. 6 (moles/hr) = 2383.72

Composition in tray no. 6 :

PROPANE = 0.23200E-2

ISOBUTANE = 0.11000E-1

N-BUTANE = 0.83960E-1

ISOPENTANE = 0.26832

N-PENTANE = 0.29861

N-HEXANE = 0.33578

**** Initial Conditions ****

Temperature in tray no. 7 (F) = 244.04

Liquid flow rate in tray no. 7 (moles/hr) = 2357.61

Composition in tray no. 7 :

PROPANE = 0.61900E-2

ISOBUTANE = 0.17510E-1

N-BUTANE = 0.11214

ISOPENTANE = 0.25552

N-PENTANE = 0.27885

N-HEXANE = 0.32978

**** Initial Conditions ****

Temperature in tray no. 8 (F) = 235.58

Liquid flow rate in tray no. 8 (moles/hr) = 2318.68

Composition in tray no. 8 :

PROPANE = 0.15910E-1

ISOBUTANE = 0.26590E-1

N-BUTANE = 0.14209

ISOPENTANE = 0.23520

N-PENTANE = 0.25568

N-HEXANE = 0.32452

**** Initial Conditions ****

Temperature in tray no. 9 (F) = 223.52

Liquid flow rate in tray no. 9 (moles/hr) = 2261.31

Composition in tray no. 9 :

PROPANE = 0.38730E-1

ISOBUTANE = 0.37720E-1

N-BUTANE = 0.16720

ISOPENTANE = 0.20764

N-PENTANE = 0.22923

N-HEXANE = 0.31947

**** Initial Conditions ****

Temperature in tray no. 10 (F) = 211.28

Liquid flow rate in tray no. 10 (moles/hr) = 918.85

Composition in tray no. 10 :

PROPANE = 0.41350E-1

ISOBUTANE = 0.41970E-1

N-BUTANE = 0.19099

ISOPENTANE = 0.28603

N-PENTANE = 0.27468

N-HEXANE = 0.16498

**** Initial Conditions ****

Temperature in tray no. 11 (F) = 204.08

Liquid flow rate in tray no. 11 (moles/hr) = 976.06

Composition in tray no. 11 :

PROPANE = 0.43060E-1

ISOBUTANE = 0.44880E-1

N-BUTANE = 0.20845

ISOPENTANE = 0.34472

N-PENTANE = 0.28590

N-HEXANE = 0.72990E-1

**** Initial Conditions ****

Temperature in tray no. 12 (F) = 200.12

Liquid flow rate in tray no. 12 (moles/hr) = 1011.21

Composition in tray no. 12 :

PROPANE = 0.44110E-1

ISOBUTANE = 0.46840E-1

N-BUTANE = 0.22198

ISOPENTANE = 0.38375

N-PENTANE = 0.27382

N-HEXANE = 0.29500E-1

**** Initial Conditions ****

Temperature in tray no. 13 (F) = 197.42

Liquid flow rate in tray no. 13 (moles/hr) = 1029.37

Composition in tray no. 13 :

PROPANE = 0.44890E-1

ISOBUTANE = 0.48520E-1

N-BUTANE = 0.23563

ISOPENTANE = 0.40906

N-PENTANE = 0.25055

N-HEXANE = 0.11340E-1

**** Initial Conditions ****

Temperature in tray no. 14 (F) = 195.08

Liquid flow rate in tray no. 14 (moles/hr) = 1038.91

Composition in tray no. 14 :

PROPANE = 0.45670E-1

ISOBUTANE = 0.50440E-1

N-BUTANE = 0.25291

ISOPENTANE = 0.42411

N-PENTANE = 0.22265

N-HEXANE = 0.42200E-2

**** Initial Conditions ****

Temperature in tray no. 15 (F) = 192.56

Liquid flow rate in tray no. 15 (moles/hr) = 1045.16

Composition in tray no. 15 :

PROPANE = 0.46620E-1

ISOBUTANE = 0.52980E-1

N-BUTANE = 0.27698

ISOPENTANE = 0.42909

N-PENTANE = 0.19280

N-HEXANE = 0.15200E-2

**** Initial Conditions ****

Temperature in tray no. 16 (F) = 189.32

Liquid flow rate in tray no. 16 (moles/hr) = 1051.09

Composition in tray no. 16 :

PROPANE = 0.47870E-1

ISOBUTANE = 0.56520E-1

N-BUTANE = 0.31088

ISOPENTANE = 0.42210

N-PENTANE = 0.16209

N-HEXANE = 0.53214E-3

**** Initial Conditions ****

Temperature in tray no. 17 (F) = 185.18

Liquid flow rate in tray no. 17 (moles/hr) = 1058.58

Composition in tray no. 17 :

PROPANE = 0.49490E-1

ISOBUTANE = 0.61440E-1

N-BUTANE = 0.35719

ISOPENTANE = 0.40050

N-PENTANE = 0.13121

N-HEXANE = 0.17765E-3

**** Initial Conditions ****

Temperature in tray no. 18 (F) = 180.14

Liquid flow rate in tray no. 18 (moles/hr) = 1069.19

Composition in tray no. 18 :

PROPANE = 0.51510E-1

ISOBUTANE = 0.68040E-1

N-BUTANE = 0.41671

ISOPENTANE = 0.36255

N-PENTANE = 0.10112

N-HEXANE = 0.56000E-4

**** Initial Conditions ****

Temperature in tray no. 19 (F) = 174.56

Liquid flow rate in tray no. 19 (moles/hr) = 1084.07

Composition in tray no. 19 :

PROPANE = 0.53920E-1

ISOBUTANE = 0.76500E-1

N-BUTANE = 0.48680

ISOPENTANE = 0.30943

N-PENTANE = 0.73330E-1

N-HEXANE = 0.16444E-4

**** Initial Conditions ****

Temperature in tray no. 20 (F) = 168.98

Liquid flow rate in tray no. 20 (moles/hr) = 1103.20

Composition in tray no. 20 :

PROPANE = 0.56720E-1

ISOBUTANE = 0.86780E-1

N-BUTANE = 0.56034

ISOPENTANE = 0.24661

N-PENTANE = 0.49550E-1

N-HEXANE = 0.44520E-5

**** Initial Conditions ****

Temperature in tray no. 21 (F) = 163.76

Liquid flow rate in tray no. 21 (moles/hr) = 1124.78

Composition in tray no. 21 :

PROPANE = 0.60210E-1

ISOBUTANE = 0.98770E-1

N-BUTANE = 0.62729

ISOPENTANE = 0.18266

N-PENTANE = 0.31070E-1

N-HEXANE = 0.11078E-5

**** Initial Conditions ****

Temperature in tray no. 22 (F) = 159.08

Liquid flow rate in tray no. 22 (moles/hr) = 1145.69

Composition in tray no. 22 :

PROPANE = 0.65750E-1

ISOBUTANE = 0.11254

N-BUTANE = 0.67784

ISOPENTANE = 0.12578

N-PENTANE = 0.18100E-1

N-HEXANE = 0.25452E-6

**** Initial Conditions ****

Temperature in tray no. 23 (F) = 154.40

Liquid flow rate in tray no. 23 (moles/hr) = 2364.0

Composition in tray no. 23 :

PROPANE = 0.77530E-1

ISOBUTANE = 0.12824

N-BUTANE = 0.70388

ISOPENTANE = 0.80540E-1

N-PENTANE = 0.98100E-2

N-HEXANE = 0.54373E-7

**** Initial Conditions ****

Temperature in tray no. 24 (F) = 148.46

Liquid flow rate in tray no. 24 (moles/hr) = 1173.29

Composition in tray no. 24 :

PROPANE = 0.10685

ISOBUTANE = 0.14526

N-BUTANE = 0.69558

ISOPENTANE = 0.47410E-1

N-PENTANE = 0.48900E-2

N-HEXANE = 0.10765E-7

**** Initial Conditions ****

Temperature in tray no. 25 (F) = 137.84

Liquid flow rate in tray no. 25 (moles/hr) = 1170.40

Composition in tray no. 25 :

PROPANE = 0.18133

ISOBUTANE = 0.15923

N-BUTANE = 0.63291

ISOPENTANE = 0.24400E-1

N-PENTANE = 0.21300E-2

N-HEXANE = 0.18784E-8

**** Initial Conditions ****

Temperature in reflux drum TD, (F) = 290.66

Composition in reflux drum :

PROPANE = 0.35394

ISOBUTANE = 0.15614

N-BUTANE = 0.48014

ISOPENTANE = 0.91300E-2

N-PENTANE = 0.65312E-3

N-HEXANE = 0.21086E-9

Press ENTER to continue


```
**** MAIN MENU ****

0) Exit to Dos
1) Components Database
2) Characteristic of Column
3) Operating Conditions
4) Feed Data
5) Initial Conditions
6) Edit Input Data
7) Save Input data
8) Run
9) Reporting & Reviewing the results

Please ENTER your selection : 8
```

Step 3 : Output of Results

After the run selection from main menu the results for each time appeared in the RESULT.DAT file and it can be printout by using an editor programming. The following are some of example results data for time 0.000 and time 0.019.

```
**** MAIN MENU ****

0) Exit to Dos
1) Components Database
2) Characteristic of Column
3) Operating Conditions
4) Feed Data
5) Initial Conditions
6) Edit Input Data
7) Save Input data
8) Run
9) Reporting & Reviewing the results

Please ENTER your selection : 9
```

TIME	T	X1	X2	X3	X4	X5	X6	L
.0000	745.15	.000003	.000244	.004760	.135850	.220110	.639040	639.140300
1	734.09	.000011	.000581	.009830	.191530	.283230	.514820	2364.000000
2	726.53	.000035	.001180	.017270	.232310	.317370	.431840	2387.700000
3	721.25	.000105	.002210	.027630	.257640	.328580	.383870	2403.500000
4	717.16	.000301	.003910	.041700	.270400	.325630	.358060	2407.020000
5	713.22	.000846	.006660	.060310	.273470	.314610	.344110	2400.120000
6	708.47	.002320	.011000	.083960	.268320	.298610	.335780	2383.720000
7	702.51	.006190	.017510	.112140	.255520	.278850	.329780	2357.610000
8	694.39	.015910	.026590	.142090	.235200	.255680	.324520	2318.680000
9	682.59	.038730	.037720	.167200	.207640	.229230	.319470	2261.310000
10	670.75	.041350	.041970	.190990	.286030	.274680	.164980	918.850000
11	663.86	.043060	.044880	.208450	.344720	.285900	.072990	976.060000
12	659.74	.044110	.046840	.221980	.383750	.273820	.029500	1011.210000
13	657.12	.044890	.048520	.235630	.409060	.250550	.011340	1029.370000
14	654.72	.045670	.050440	.252910	.424110	.222650	.004220	1038.910000
15	652.15	.046620	.052980	.276980	.429090	.192800	.001520	1045.160000
16	648.77	.047870	.056520	.310880	.422100	.162090	.000532	1051.090000
17	644.51	.049490	.061440	.357190	.400500	.131210	.000178	1058.580000
18	639.40	.051510	.068040	.416710	.362550	.101120	.000056	1069.190000
19	633.69	.053920	.076500	.486800	.309430	.073330	.000016	1084.070000
20	627.89	.056720	.086780	.560340	.246610	.049550	.000004	1103.200000
21	622.51	.060210	.098770	.627290	.182660	.031070	.000001	1124.780000
22	617.70	.065750	.112540	.677840	.125780	.018100	.000000	1145.690000
23	613.02	.077530	.128240	.703880	.080540	.009810	.000000	1162.670000
24	606.94	.106850	.145260	.695580	.047410	.004890	.000000	1173.290000
25	596.34	.181330	.159230	.632910	.024400	.002130	.000000	1177.400000
	577.09	.353940	.156140	.480140	.009130	.000653	.000000	1800.000000
		.583560	.123000	.290687	.002602	.000152	.000000	253.293700

TIME	T	X1	X2	X3	X4	X5	X6	L
.0191	742.56	.000005	.000358	.006194	.150874	.232981	.609589	1116.407000
1	731.70	.000018	.000860	.012906	.205799	.290549	.489863	2730.133000
2	724.14	.000054	.001694	.022234	.244559	.321198	.410254	2661.987000
3	718.27	.000146	.003022	.034745	.270716	.333883	.357482	2572.897000
4	713.26	.000377	.005080	.051088	.286317	.334305	.322828	2476.628000
5	708.64	.000923	.008086	.071144	.292671	.326484	.300688	2382.223000
6	704.08	.002138	.012193	.093965	.291342	.313679	.286677	2288.135000
7	699.40	.004637	.017332	.117334	.284078	.298473	.278141	2196.655000
8	694.50	.009256	.023020	.137786	.273186	.283190	.273555	2105.747000
9	689.58	.016718	.028314	.151670	.261895	.270145	.271250	2025.836000
10	682.79	.015246	.028660	.161508	.323772	.304233	.166577	863.983900
11	677.64	.014489	.030018	.174342	.370891	.312725	.097530	962.216900
12	673.53	.013748	.031968	.189951	.409850	.303596	.050881	1111.204000
13	669.78	.013318	.034795	.210252	.437988	.279903	.023739	1318.883000
14	665.83	.013554	.038956	.238656	.452410	.246373	.010049	1566.764000
15	661.16	.014715	.044830	.278537	.450296	.207697	.003922	1804.034000
16	655.32	.017033	.052670	.332077	.429359	.167437	.001424	1982.990000
17	648.37	.020761	.062563	.399011	.388914	.128270	.000482	2094.505000
18	640.94	.026144	.074422	.475202	.331499	.092583	.000151	2150.718000
19	633.17	.033702	.088083	.552221	.263534	.062416	.000044	2181.102000
20	625.83	.044553	.103235	.618668	.194424	.039109	.000012	2193.337000
21	618.99	.061172	.119358	.663573	.133118	.022777	.000003	2184.994000
22	611.86	.088208	.135474	.679174	.084789	.012356	.000001	2150.055000
23	604.05	.132355	.149666	.661453	.050290	.006238	.000000	2072.359000
24	594.53	.199224	.158847	.611147	.027860	.002924	.000000	1966.329000
25	584.32	.285118	.159954	.538612	.015001	.001316	.000000	1863.649000
	575.84	.368460	.153256	.468322	.009263	.000701	.000000	1800.000000
		.599613	.118836	.278803	.002589	.000160	.000000	-950.767400

Tables 4.3 and 4.4 summarize the composition responses of top and bottom and top stages in various times for dynamic distillation.

Table 4.3 Reboiler compositions in various times.

REBOILER COMPOSITIONS FOR 100% FEED

TIME	T	X1	X2	X3	X4	X5	X6
0.000	745.15	0.000003	0.000244	0.004760	0.135850	0.220110	0.639040
0.001	745.15	0.000003	0.000242	0.004714	0.136444	0.220656	0.637950
0.002	745.15	0.000003	0.000238	0.004648	0.136476	0.220537	0.638107
0.003	745.15	0.000003	0.000234	0.004580	0.136248	0.220128	0.638819
0.004	745.31	0.000003	0.000229	0.004494	0.135783	0.219434	0.640071
0.005	745.46	0.000003	0.000223	0.004402	0.135174	0.218563	0.641650
0.006	745.46	0.000003	0.000219	0.004323	0.134591	0.217739	0.643142
0.007	745.63	0.000003	0.000216	0.004270	0.134156	0.217080	0.644293
0.008	745.79	0.000002	0.000215	0.004231	0.133817	0.216531	0.645222
0.009	745.79	0.000002	0.000215	0.004224	0.133737	0.216268	0.645572
0.010	745.79	0.000002	0.000217	0.004246	0.133910	0.216288	0.645354
0.011	745.79	0.000002	0.000221	0.004288	0.134322	0.216577	0.644606
0.012	745.63	0.000002	0.000226	0.004365	0.135064	0.217228	0.643130
0.013	745.47	0.000003	0.000235	0.004490	0.136244	0.218355	0.640687
0.014	745.10	0.000003	0.000248	0.004664	0.137861	0.219955	0.637282
0.015	744.73	0.000003	0.000263	0.004879	0.139842	0.221941	0.633081
0.016	744.19	0.000003	0.000282	0.005148	0.142218	0.224334	0.628022
0.017	743.62	0.000004	0.000304	0.005462	0.144907	0.227038	0.622290
0.018	743.10	0.000004	0.000330	0.005812	0.147808	0.229939	0.616110
0.019	742.56	0.000005	0.000358	0.006194	0.150874	0.232981	0.609589

Table 4.4 Distillate compositions in various times.**DISTILLATE COMPOSITIONS FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.001	575.97	0.366578	0.153489	0.469907	0.009323	0.000705	0.000000
0.002	576.22	0.364789	0.153709	0.471416	0.009379	0.000709	0.000000
0.003	576.35	0.363100	0.153916	0.472843	0.009430	0.000713	0.000000
0.004	576.48	0.361490	0.154115	0.474205	0.009476	0.000716	0.000000
0.005	576.59	0.359959	0.154307	0.475502	0.009517	0.000718	0.000000
0.006	576.84	0.358557	0.154487	0.476690	0.009549	0.000719	0.000000
0.007	576.97	0.356182	0.154819	0.478701	0.009582	0.000718	0.000000
0.008	576.97	0.357296	0.154657	0.477759	0.009571	0.000719	0.000000
0.009	577.09	0.353940	0.156140	0.480140	0.009130	0.000653	0.000000
0.010	577.09	0.355236	0.154974	0.479495	0.009580	0.000716	0.000000
0.011	577.22	0.353527	0.156063	0.480566	0.009187	0.000660	0.000000
0.012	577.22	0.353296	0.155970	0.480829	0.009241	0.000666	0.000000
0.013	577.22	0.353168	0.155876	0.480995	0.009291	0.000672	0.000000
0.014	577.22	0.353096	0.155765	0.481115	0.009347	0.000679	0.000000
0.015	577.22	0.353114	0.155638	0.481156	0.009407	0.000687	0.000000
0.016	577.22	0.353241	0.155517	0.481092	0.009458	0.000694	0.000000
0.017	577.22	0.353498	0.155391	0.480910	0.009503	0.000701	0.000000
0.018	577.22	0.353904	0.155259	0.480592	0.009540	0.000707	0.000000
0.019	577.22	0.354479	0.155120	0.480125	0.009566	0.000712	0.000000

Example 2 : Dynamic compartmental

Given : Using the same data from example 1 (Table 4.1) but applied by the compartmental technique with five-compartmental model.

Compartmental Configuration : The five-compartmental model was constructed by using a guideline of Benallou et al (1986) that the sensitive tray of each compartment is taken midway between the first and last stages in the compartment. First, it is divided at a feed tray location, 9th stage, and used as a feed compartment, f . The lower section, 1st through 8th stage, is called stripping section while the upper section, 10th through 25th stage, is called rectifying section. It can be grouped into two compartments by dividing the stages in each section, therefore, the first compartment

consist of 1st through 3rd stage, the second compartment consist of 4th through 8th stage, the third compartment consist of only 9th stage, the fourth compartment consist of 10th through 18th stage, and the last, the fifth compartment, consist of 19th through 25th stage. With a guideline of Benallou et al, the sensitive stages in each compartment are taken midway between first and last stage in each compartment, i.e., 2nd, 6th, 9th, 15th, and 22nd respectively. Note that the reboiler and condenser are not include in the number of compartment but can be calculated by the same equation of a full-order model. The configuration of this example is shown in Figure 4.1. Table 4.5 shows the given compartmentation parameters data.

Table 4.5 Compartmentation Parameters (Five-compartment Model)

Data for Example 2.

$k = 5$	$r1 = 3$	$s1 = 2$	$t1 = 1$	$f = 3$
	$r2 = 8$	$s2 = 6$	$t2 = 4$	
	$r3 = 9$	$s3 = 9$	$t3 = 9$	
	$r4 = 18$	$s4 = 15$	$t4 = 10$	
	$r5 = 25$	$s5 = 22$	$t5 = 19$	

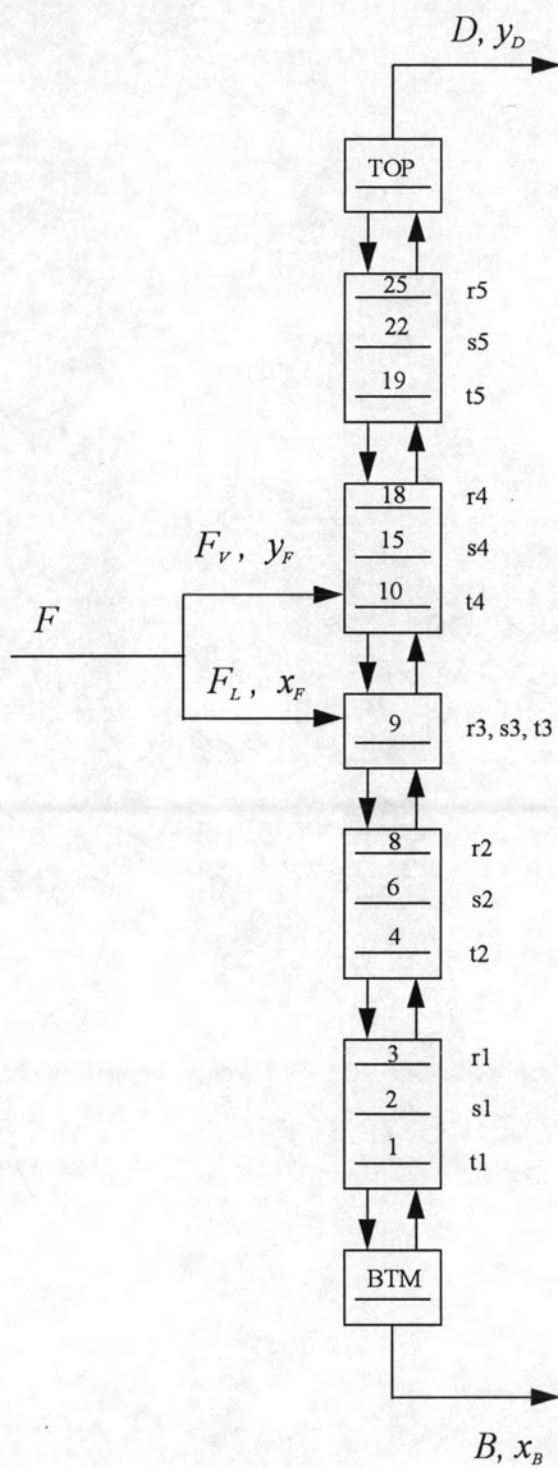


Figure 4.1 Distillation column compartmentation, five compartments.

(Excluding TOP and BTM stage)

Original results : Using the same original results from example 1 (Table 4.2) because there were not have anything changed but only applied by compartmental technique.

Program Execution :

Step 1 : Start-up procedure

Load the working program by typing the working file name.

A> DYNAMICS

Step 2 : Input data

Select number 6 from main menu to obtain old data from example 1 (filename EX1.DAT). After edit an old data, select number 2 from main menu and input a compartmentation parameter as follow:

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25

Number of trays in stripping section (NF) = 9

Weir height in stripping section (WHS) = 3.44

Weir height in rectifying section (WHR) = 3.44

Column diameter in stripping section (DS) = 72.0

Column diameter in rectifying section (DR) = 72.0

Weir length in stripping section (WLS) = 51.1

Weir length in rectifying section (WLR) = 51.1

Volumetric holdup in column base (MVB) = 130.0

Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : Y

Press ENTER to continue

**** Characteristic of Compartment ****

Number of Compartment, k = 5

Feed Compartment, f = 3

r1 = 3 s1 = 2 t1 = 1

r2 = 8 s2 = 6 t2 = 4

r3 = 9 s3 = 9 t3 = 9

r4 = 18 s4 = 15 t4 = 10

r5 = 25 s5 = 22 t5 = 19

Press ENTER to continue

```
**** MAIN MENU ****

0) Exit to Dos
1) Components Database
2) Characteristic of Column
3) Operating Conditions
4) Feed Data
5) Initial Conditions
6) Edit Input Data
7) Save Input data
8) Run
9) Reporting & Reviewing the results

Please ENTER your selection : 8
```

Step 3 : Output of Results

After the run selection from main menu the results for each time appeared in the RESULTC.DAT file and it can be printout by using an editor programming. The following are some of example results data for time 0.000 and time 0.014.

```
**** MAIN MENU ****

0) Exit to Dos
1) Components Database
2) Characteristic of Column
3) Operating Conditions
4) Feed Data
5) Initial Conditions
6) Edit Input Data
7) Save Input data
8) Run
9) Reporting & Reviewing the results

Please ENTER your selection : 9
```

TIME	T	X1	X2	X3	X4	X5	X6	L
.0000	745.15	.000003	.000244	.004760	.135850	.220110	.639040	639.1
2	726.53	.000035	.001180	.017270	.232310	.317370	.431840	2387.7
6	708.47	.002320	.011000	.083960	.268320	.298610	.335780	2383.7
9	682.59	.038730	.037720	.167200	.207640	.229230	.319470	2261.3
15	652.15	.046620	.052980	.276980	.429090	.192800	.001520	1045.2
22	617.70	.065750	.112540	.677840	.125780	.018100	.000000	1145.7
	577.09	.353940	.156140	.480140	.009130	.000653	.000000	1800.0
		.583560	.123000	.290687	.002602	.000152	.000000	253.3

TIME	T	X1	X2	X3	X4	X5	X6	L
.0141	743.98	.000003	.000260	.005006	.142298	.227656	.624785	1043.1
2	731.34	.000029	.000856	.012281	.231165	.321144	.385447	2658.3
6	706.52	.001607	.008233	.063846	.283121	.324238	.372067	2167.9
9	687.69	.023979	.032272	.158437	.236461	.252515	.296327	1662.4
15	659.45	.001455	.028325	.398664	.404417	.135793	.000760	1048.5
22	611.95	.023487	.169402	.833567	.014626	.001416	.000000	1980.0
	577.69	.348034	.155744	.485833	.009678	.000712	.000000	1800.0
		.577149	.123554	.296348	.002782	.000168	.000000	-866.9

Tables 4.6 and 4.7 summarize the composition responses of top and bottom and top stages in various times for a dynamic compartmental model. However, the composition responses in the intermediate stages, sensitive trays in each compartment, can be summarized in Tables 4.8 through 4.12 respectively.

Table 4.6 Reboiler composition in various times using compartmental technique.

**REBOILER COMPOSITIONS USING
COMPARTMENTAL TECHNIQUE FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	745.15	0.000003	0.000244	0.004760	0.135850	0.220110	0.639040
0.001	745.15	0.000003	0.000243	0.004734	0.136627	0.220929	0.637472
0.002	745.00	0.000003	0.000241	0.004705	0.136976	0.221306	0.636777
0.003	745.00	0.000003	0.000239	0.004675	0.137061	0.221397	0.636633
0.004	745.00	0.000003	0.000237	0.004643	0.137002	0.221326	0.636797
0.005	745.00	0.000003	0.000236	0.004613	0.136850	0.221143	0.637164
0.006	745.00	0.000003	0.000235	0.004594	0.136720	0.220983	0.637474
0.007	745.00	0.000003	0.000234	0.004587	0.136672	0.220915	0.637598
0.008	745.00	0.000003	0.000235	0.004595	0.136775	0.221022	0.637379
0.009	745.00	0.000003	0.000237	0.004621	0.137090	0.221381	0.636677
0.010	745.00	0.000003	0.000240	0.004668	0.137670	0.222058	0.635370
0.011	744.83	0.000003	0.000244	0.004732	0.138504	0.223049	0.633477
0.012	744.49	0.000003	0.000249	0.004813	0.139589	0.224353	0.631002
0.013	744.32	0.000003	0.000254	0.004907	0.140882	0.225921	0.628041
0.014	743.98	0.000003	0.000260	0.005006	0.142298	0.227656	0.624785

Table 4.7 Distillate composition in various times using compartmental technique.

**DISTILLATE COMPOSITIONS USING
COMPARTMENTAL TECHNIQUE FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	577.09	0.353940	0.156140	0.480140	0.009130	0.000653	0.000000
0.001	577.21	0.353336	0.156097	0.480723	0.009188	0.000659	0.000000
0.002	577.21	0.352781	0.156059	0.481258	0.009240	0.000665	0.000000
0.003	577.33	0.352282	0.156025	0.481739	0.009287	0.000670	0.000000
0.004	577.33	0.351734	0.155988	0.482267	0.009338	0.000676	0.000000
0.005	577.45	0.351147	0.155949	0.482832	0.009392	0.000681	0.000000
0.006	577.45	0.350637	0.155916	0.483324	0.009439	0.000687	0.000000
0.007	577.57	0.350156	0.155884	0.483787	0.009483	0.000691	0.000000
0.008	577.57	0.349711	0.155855	0.484216	0.009524	0.000696	0.000000
0.009	577.57	0.349309	0.155828	0.484605	0.009561	0.000700	0.000000
0.010	577.69	0.348954	0.155805	0.484947	0.009594	0.000703	0.000000
0.011	577.69	0.348648	0.155785	0.485241	0.009622	0.000706	0.000000
0.012	577.69	0.348394	0.155768	0.485486	0.009645	0.000709	0.000000
0.013	577.69	0.348191	0.155755	0.485682	0.009663	0.000711	0.000000
0.014	577.69	0.348034	0.155744	0.485833	0.009678	0.000712	0.000000

Table 4.8 Compositions in compartment 1 for 100% feed.**COMPOSITIONS IN COMPARTMENT 1 FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	726.53	0.000035	0.001180	0.017270	0.232310	0.317370	0.431840
0.001	727.51	0.000021	0.000985	0.015162	0.225136	0.310748	0.453592
0.002	728.05	0.000013	0.000835	0.013529	0.219942	0.306652	0.470810
0.003	728.23	0.000010	0.000720	0.012237	0.216097	0.304157	0.483958
0.004	728.43	0.000008	0.000617	0.011014	0.212708	0.302509	0.495465
0.005	728.62	0.000007	0.000533	0.009925	0.209964	0.301806	0.504144
0.006	728.80	0.000007	0.000481	0.009170	0.208382	0.302062	0.508059
0.007	728.98	0.000007	0.000448	0.008635	0.207712	0.303088	0.507749
0.008	729.17	0.000008	0.000435	0.008325	0.208028	0.304826	0.502565
0.009	729.38	0.000008	0.000441	0.008255	0.209457	0.307258	0.491949
0.010	729.94	0.000010	0.000469	0.008452	0.212151	0.310364	0.475657
0.011	730.32	0.000013	0.000520	0.008923	0.215907	0.313729	0.454877
0.012	730.90	0.000017	0.000599	0.009706	0.220579	0.316974	0.430818
0.013	731.21	0.000022	0.000710	0.010828	0.225844	0.319615	0.406368
0.014	731.34	0.000029	0.000856	0.012281	0.231165	0.321144	0.385447

Table 4.9 Compositions in compartment 2 for 100% feed.**COMPOSITIONS IN COMPARTMENT 2 FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	708.47	0.002320	0.011000	0.083960	0.268320	0.298610	0.335780
0.001	709.71	0.001326	0.009665	0.078588	0.272112	0.304363	0.330882
0.002	710.73	0.000997	0.008564	0.073675	0.275737	0.309390	0.323529
0.003	711.80	0.000880	0.007720	0.069346	0.278713	0.313513	0.315681
0.004	712.86	0.000818	0.006968	0.064857	0.281467	0.317491	0.306788
0.005	713.88	0.000783	0.006351	0.060493	0.283754	0.321090	0.297737
0.006	714.76	0.000773	0.005966	0.057220	0.285179	0.323641	0.290988
0.007	715.36	0.000782	0.005738	0.054738	0.286058	0.325518	0.286385
0.008	715.65	0.000812	0.005661	0.053156	0.286493	0.326748	0.284762
0.009	715.65	0.000869	0.005734	0.052556	0.286557	0.327343	0.287055
0.010	715.03	0.000956	0.005962	0.052990	0.286257	0.327265	0.294184
0.011	713.68	0.001070	0.006330	0.054397	0.285710	0.326716	0.306438
0.012	711.76	0.001219	0.006841	0.056752	0.284948	0.325850	0.324184
0.013	709.23	0.001401	0.007484	0.059959	0.284029	0.324905	0.346690
0.014	706.52	0.001607	0.008233	0.063846	0.283121	0.324238	0.372067

Table 4.10 Compositions in compartment 3 for 100% feed.**COMPOSITIONS IN COMPARTMENT 3 FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	682.59	0.038730	0.037720	0.167200	0.207640	0.229230	0.319470
0.001	686.50	0.026449	0.034251	0.163527	0.226970	0.244175	0.304619
0.002	687.28	0.023625	0.032979	0.161805	0.234976	0.250411	0.296196
0.003	687.51	0.022773	0.032405	0.160763	0.238421	0.253278	0.292353
0.004	687.72	0.022331	0.032014	0.159788	0.240089	0.254895	0.290877
0.005	687.95	0.022038	0.031713	0.158817	0.240542	0.255630	0.291252
0.006	688.15	0.021878	0.031516	0.158051	0.240303	0.255754	0.292492
0.007	688.38	0.021782	0.031373	0.157403	0.239774	0.255594	0.294067
0.008	688.60	0.021778	0.031291	0.156923	0.239120	0.255259	0.295622
0.009	688.60	0.021888	0.031288	0.156684	0.238451	0.254818	0.296865
0.010	688.60	0.022084	0.031347	0.156628	0.237835	0.254341	0.297757
0.011	688.40	0.022384	0.031476	0.156779	0.237318	0.253860	0.298177
0.012	688.18	0.022820	0.031682	0.157158	0.236894	0.253370	0.298068
0.013	687.95	0.023353	0.031950	0.157714	0.236605	0.252917	0.297453
0.014	687.69	0.023979	0.032272	0.158437	0.236461	0.252515	0.296327

Table 4.11 Compositions in compartment 4 for 100% feed.**COMPOSITIONS IN COMPARTMENT 4 FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	652.15	0.046620	0.052980	0.276980	0.429090	0.192800	0.001520
0.001	666.38	0.003036	0.046342	0.290247	0.437843	0.179800	0.001052
0.002	666.26	0.001557	0.041542	0.302131	0.441936	0.170709	0.001205
0.003	665.64	0.001431	0.038110	0.312672	0.443836	0.164736	0.001358
0.004	664.67	0.001393	0.035167	0.324109	0.444647	0.160174	0.001533
0.005	663.31	0.001374	0.032805	0.336239	0.444611	0.157200	0.001730
0.006	662.08	0.001362	0.031285	0.346724	0.444090	0.155878	0.001889
0.007	660.82	0.001358	0.030221	0.356573	0.443183	0.155370	0.002000
0.008	659.67	0.001356	0.029495	0.365660	0.441774	0.155181	0.002047
0.009	658.71	0.001359	0.029013	0.373849	0.439561	0.154782	0.002003
0.010	658.09	0.001370	0.028707	0.381020	0.436133	0.153649	0.001849
0.011	657.81	0.001385	0.028521	0.387126	0.431173	0.151417	0.001624
0.012	657.81	0.001402	0.028411	0.392089	0.424338	0.147768	0.001341
0.013	658.46	0.001427	0.028353	0.395911	0.415413	0.142535	0.001035
0.014	659.45	0.001455	0.028325	0.398664	0.404417	0.135793	0.000760

Table 4.12 Compositions in compartment 5 for 100% feed.**COMPOSITIONS IN COMPARTMENT 5 FOR 100% FEED**

TIME	T	X1	X2	X3	X4	X5	X6
0.000	617.70	0.065750	0.112540	0.677840	0.125780	0.018100	0.000000
0.001	618.38	0.060761	0.125318	0.688858	0.090142	0.010461	0.000000
0.002	623.00	0.037220	0.134668	0.699911	0.067091	0.006526	0.000000
0.003	623.87	0.028725	0.141563	0.710678	0.051979	0.004436	0.000000
0.004	623.38	0.025261	0.147782	0.723381	0.039950	0.003089	0.000000
0.005	622.06	0.024025	0.153179	0.738000	0.030956	0.002292	0.000000
0.006	620.65	0.023651	0.157032	0.751585	0.025498	0.001911	0.000000
0.007	619.19	0.023500	0.160095	0.765138	0.021821	0.001708	0.000000
0.008	617.77	0.023430	0.162533	0.778339	0.019357	0.001599	0.000000
0.009	616.42	0.023395	0.164472	0.790832	0.017710	0.001541	0.000000
0.010	615.20	0.023384	0.166006	0.802265	0.016603	0.001508	0.000000
0.011	614.22	0.023393	0.167217	0.812418	0.015843	0.001484	0.000000
0.012	613.29	0.023414	0.168158	0.821063	0.015308	0.001463	0.000000
0.013	612.54	0.023446	0.168872	0.828093	0.014919	0.001441	0.000000
0.014	611.95	0.023487	0.169402	0.833567	0.014626	0.001416	0.000000

Table 4.13 Compartmentation Parameters (Four-compartment Model)

$k = 4$	$r1 = 3$	$s1 = 2$	$t1 = 1$	$f = 3$
	$r2 = 8$	$s2 = 6$	$t2 = 4$	
	$r3 = 9$	$s3 = 9$	$t3 = 9$	
	$r4 = 25$	$s4 = 22$	$t4 = 10$	

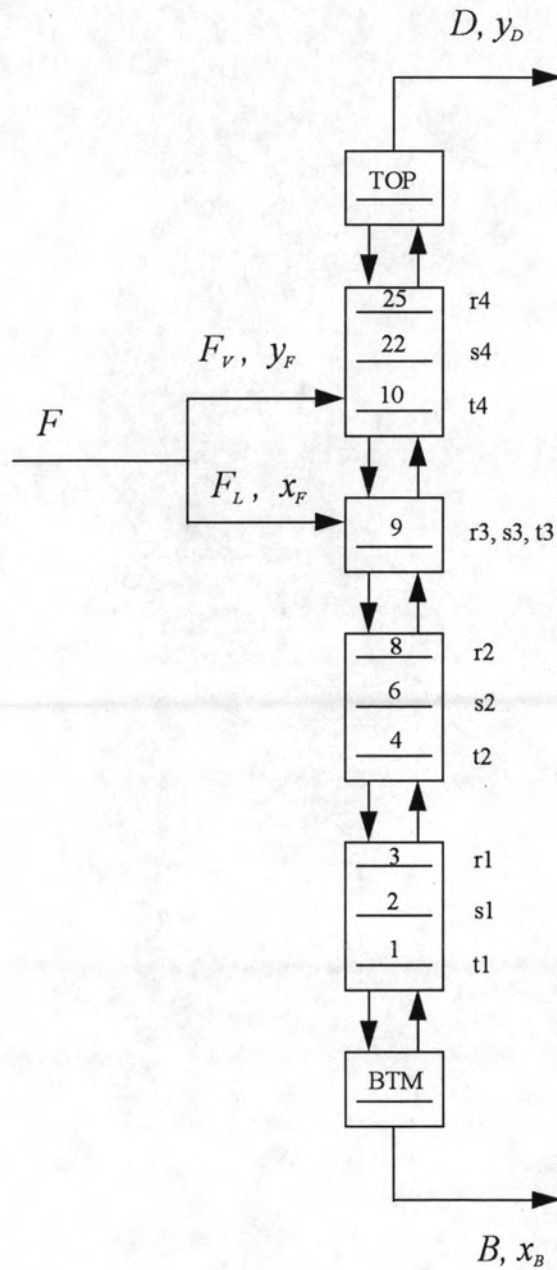


Figure 4.3 Distillation column compartmentation, four compartments.
(Excluding TOP and BTM stage)

4.2 Application to an oil refinery

In order to illustrate the dynamic compartmental approach, the Debutanizer of Bangchak Petroleum Industry Company Limited was selected as our column case study, Figure 4.2 (3C-402). A $\pm 15\%$ step change in feed flow rate has considered in the same way as the previous section. To compare the behaviour of each case, a five-compartment, which constructed by taking midway between first and last stages as a sensitive tray in compartment as shown in Figure 4.1 and Table 4.5, have been used to simulate against a full-order model at the same conditions. Furthermore, another compartmental model, four-compartment, have been constructed to study the different of compartment selection. The four-compartmental model was followed to a guideline of Horton (1990) by taking the upper portion of the fourth-compartment in rectifying section, approximately one-quarter of the way down, as a sensitive tray in that compartment, therefore, in the rectifying section of four-compartmental model, it can be grouped the stages in these section into one compartment and selected approximately one-quarter of the way down, 22nd stage, as the sensitive tray as shown in Figure 4.3 and Table 4.13 while the stripping section sensitive trays are the same as a five-compartmental model because this column has a lower feed location and can not have a distinction. Finally, the comparisons with the existing steady state data that obtained from the steady state program, PRO II, are also considered to verify the reliability of the program.

4.2.1 Application to +15% step changes in feed flow rate

First, using the Dynamic Simulation Software introduced in the previous chapter to calculate the behaviour of distillation column, called the full-order model. The data changed from Example 1 and 2 are shown in Table 4.14 for +15% step change in feed flow rate. Then the compartmental model was applied using both

guidelines of Benallou et al and Horton to simulate the behaviour of the same column comparing with full-order model.

Table 4.14 Feed Data for +15% Change.

Feed Data								
Phase	Temp. (°F)	Feed Flowrate (lbmole/hr)	Propane X_1	Isobutane X_2	N-Butane X_3	Isopentane X_4	N-Pentane X_5	N-Hexane X_6
Liquid	233.60	1452.58	.38730E-1	.37720E-1	.16720	.20764	.22923	.31947
Vapour	233.60	2.19	.13531	.75961E-1	.27746	.19462	.18776	.12889

4.2.1.1 Running a full-order model

Edit the old data from EX1.DAT by selecting number 6 of main menu, input the feed changes, and save the input data before running the program as follows:

A> DYNAMICS



**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX1.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 4

**** Feed Data ****

Liquid Feed flow rate (moles/hr) = 1452.58

Liquid Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.038730

ISOBUTANE = 0.037720

N-BUTANE = 0.16720

ISOPENTANE = 0.20764

N-PENTANE = 0.22923

N-HEXANE = 0.31947

**** Feed Data ****

Vapor Feed flow rate (moles/hr) = 2.19

Vapor Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.135310

ISOBUTANE = 0.075961

N-BUTANE = 0.277460

ISOPENTANE = 0.194620

N-PENTANE = 0.187760

N-HEXANE = 0.128890

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX3.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8


```
**** RUN MENU ****

0) Return to Main Menu
1) Running a full-order model
2) Running a compartmental model

Please ENTER your selection : 1
```

4.2.1.2 Running a five-compartmental model

Edit the old data from EX3.DAT by selecting number 6 of main menu, input the characteristic of a compartment as Table 4.5, and save the input data to a new filename, EX4.DAT, before running the program.

A> DYNAMICS

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX3.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25
 Number of trays in stripping section (NF) = 9
 Weir height in stripping section (WHS) = 3.44
 Weir height in rectifying section (WHR) = 3.44
 Column diameter in stripping section (DS) = 72.0
 Column diameter in rectifying section (DR) = 72.0
 Weir length in stripping section (WLS) = 51.1
 Weir length in rectifying section (WLR) = 51.1
 Volumetric holdup in column base (MVB) = 130.0
 Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : Y
 Press ENTER to continue

**** Characteristic of Compartment ****

Number of Compartment, k = 5
 Feed Compartment, f = 3
 r1 = 3 s1 = 2 t1 = 1
 r2 = 8 s2 = 6 t2 = 4
 r3 = 9 s3 = 9 t3 = 9
 r4 = 18 s4 = 15 t4 = 10
 r5 = 25 s5 = 22 t5 = 19

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX4.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8

```
**** RUN MENU ****

0) Return to Main Menu
1) Running a full-order model
2) Running a compartmental model

Please ENTER your selection : 2
```

4.2.1.3 Running a four-compartmental model

Edit the old data from EX4.DAT by selecting number 6 of main menu, input the new characteristic of a compartment as Table 4.13, and save the input data to a new filename, EX5.DAT, before running the program.

A> DYNAMICS



**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX4.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25
 Number of trays in stripping section (NF) = 9
 Weir height in stripping section (WHS) = 3.44
 Weir height in rectifying section (WHR) = 3.44
 Column diameter in stripping section (DS) = 72.0
 Column diameter in rectifying section (DR) = 72.0
 Weir length in stripping section (WLS) = 51.1
 Weir length in rectifying section (WLR) = 51.1
 Volumetric holdup in column base (MVB) = 130.0
 Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : Y

Press ENTER to continue

**** Characteristic of Compartment ****

Number of Compartment, k = 4
 Feed Compartment, f = 3
 r1 = 3 s1 = 2 t1 = 1
 r2 = 8 s2 = 6 t2 = 4
 r3 = 9 s3 = 9 t3 = 9
 r4 = 25 s4 = 22 t4 = 10

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX5.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8

```
**** RUN MENU ****  
  
0) Return to Main Menu  
1) Running a full-order model  
2) Running a compartmental model  
  
Please ENTER your selection : 2
```

The results of above calculations are compared with a full-order model, a five-compartmental model and a four-compartmental model as shown by considering the composition's responses of n-Butane, a desirable component, in top and bottom stages. In Tables 4.15 and 4.16 the dynamic responses of the top and bottom stages for +15% step change in feed flow rate are summarized.

Table 4.15 Distillate composition response to a +15% step change in feed flow rate.

**DISTILLATE PRODUCT WITH 115% FEED
(N-BUTANE)**

TIME	FULL-ORDER	FIVE (5) COMPARTMENT	FOUR (4) COMPARTMENT
0.0000	0.480140	0.480140	0.480140
0.0011	0.480821	0.480807	0.480810
0.0021	0.481524	0.481410	0.481409
0.0031	0.482203	0.481949	0.481945
0.0041	0.482959	0.482534	0.482525
0.0051	0.483742	0.483156	0.483150
0.0061	0.484377	0.483694	0.483690
0.0071	0.484893	0.484200	0.484198
0.0081	0.485283	0.484669	0.484668
0.0091	0.485495	0.485095	0.485097
0.0101	0.485519	0.485476	0.485479
0.0111	0.485630	0.485808	0.485812
0.0121	0.485696	0.485808	0.485812
0.0131	0.485732	0.485808	0.485812
0.0141	0.485800	0.485808	0.485812

Table 4.16 Bottom composition response to a +15% step change in feed flow rate.

**BOTTOM PRODUCT WITH 115% FEED
(N-BUTANE)**

TIME	FULL-ORDER	FIVE (5) COMPARTMENT	FOUR (4) COMPARTMENT
0.0000	0.004760	0.00476	0.00476
0.0011	0.004713	0.004529	0.004499
0.0021	0.004641	0.004333	0.004273
0.0031	0.004567	0.00418	0.004092
0.0041	0.004481	0.004044	0.003925
0.0051	0.004391	0.003934	0.003784
0.0061	0.004318	0.003869	0.003697
0.0071	0.004256	0.003832	0.003647
0.0081	0.004212	0.003822	0.003631
0.0091	0.004193	0.003835	0.003643
0.0101	0.004197	0.003867	0.003679
0.0111	0.004227	0.003911	0.003731
0.0121	0.004294		0.003792
0.0131	0.004403		
0.0141	0.004555		

4.2.2 Application to -15% step changes in feed flow rate

In order to test the robustness of the results, the reduced of 15% in feed flow rate are considered. The data changed from the previous section are shown in Table 4.17 and the calculations have followed to the same steps.

Table 4.17 Feed Data for -15% Change.

Feed Data								
Phase	Temp. (°F)	Feed Flowrate (lbmole/hr)	Propane X ₁	Isobutane X ₂	N-Butane X ₃	Isopentane X ₄	N-Pentane X ₅	N-Hexane X ₆
Liquid	233.60	1073.64	.38730E-1	.37720E-1	.16720	.20764	.22923	.31947
Vapour	233.60	1.62	.13531	.75961E-1	.27746	.19462	.18776	.12889

4.2.2.1 Running a full-order model

Edit the old data from EX3.DAT by selecting number 6 of main menu, input the feed changes, and save the input data into a new filename, EX6.DAT, before running the program.

A> DYNAMICS

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX3.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 4

**** Feed Data ****

Liquid Feed flow rate (moles/hr) = 1073.64

Liquid Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.038730

ISOBUTANE = 0.037720

N-BUTANE = 0.16720

ISOPENTANE = 0.20764

N-PENTANE = 0.22923

N-HEXANE = 0.31947

**** Feed Data ****

Vapor Feed flow rate (moles/hr) = 1.62

Vapor Feed temperature (F) = 233.60

Composition (mole fraction) :

PROPANE = 0.135310

ISOBUTANE = 0.075961

N-BUTANE = 0.277460

ISOPENTANE = 0.194620

N-PENTANE = 0.187760

N-HEXANE = 0.128890

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX6.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8



```
**** RUN MENU ****

0) Return to Main Menu
1) Running a full-order model
2) Running a compartmental model

Please ENTER your selection : 1
```

4.2.2.2 Running a five-compartmental model

Edit the old data from EX6.DAT by selecting number 6 of main menu, input the characteristic of a compartment as Table 4.5, and save the input data to a new filename, EX7.DAT, before running the program.

A> DYNAMICS

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX6.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25

Number of trays in stripping section (NF) = 9

Weir height in stripping section (WHS) = 3.44

Weir height in rectifying section (WHR) = 3.44

Column diameter in stripping section (DS) = 72.0

Column diameter in rectifying section (DR) = 72.0

Weir length in stripping section (WLS) = 51.1

Weir length in rectifying section (WLR) = 51.1

Volumetric holdup in column base (MVB) = 130.0

Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : Y

Press ENTER to continue

**** Characteristic of Compartment ****

Number of Compartment, k = 5

Feed Compartment, f = 3

r1 = 3 s1 = 2 t1 = 1

r2 = 8 s2 = 6 t2 = 4

r3 = 9 s3 = 9 t3 = 9

r4 = 18 s4 = 15 t4 = 10

r5 = 25 s5 = 22 t5 = 19

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX7.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8


```
**** RUN MENU ****  
  
0) Return to Main Menu  
1) Running a full-order model  
2) Running a compartmental model  
  
Please ENTER your selection : 2
```

4.2.2.3 Running a four-compartmental model

Edit the old data from EX7.DAT by selecting number 6 of main menu, input the new characteristic of a compartment as Table 4.13, and save the input data to a new filename, EX8.DAT, before running the program.

A> DYNAMICS

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 6

*** Edit Old Data ***

Please type data file name : EX7.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 2

**** Characteristic of Column ****

Total number of plates (NT) = 25
 Number of trays in stripping section (NF) = 9
 Weir height in stripping section (WHS) = 3.44
 Weir height in rectifying section (WHR) = 3.44
 Column diameter in stripping section (DS) = 72.0
 Column diameter in rectifying section (DR) = 72.0
 Weir length in stripping section (WLS) = 51.1
 Weir length in rectifying section (WLR) = 51.1
 Volumetric holdup in column base (MVB) = 130.0
 Volumetric holdup in reflux drum (MVD) = 98.0

Do you need to input a Characteristic of compartment? (Y/N) : Y

Press ENTER to continue

**** Characteristic of Compartment ****

Number of Compartment, k = 4
 Feed Compartment, f = 3
 r1 = 3 s1 = 2 t1 = 1
 r2 = 8 s2 = 6 t2 = 4
 r3 = 9 s3 = 9 t3 = 9
 r4 = 25 s4 = 22 t4 = 10

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 7

*** Save Data ***

Please type data file name : EX8.DAT

Press ENTER to continue

**** MAIN MENU ****

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : 8

```
**** RUN MENU ****  
  
0) Return to Main Menu  
1) Running a full-order model  
2) Running a compartmental model  
  
Please ENTER your selection : 2
```

Again, the results of above calculations are compared with a full-order model, a five-compartmental model and a four-compartmental model as shown by considering the composition's responses of n-Butane, the desirable component, in top and bottom stages. In Tables 4.18 and 4.19 the dynamic responses of the top and bottom stages for -15% step change in feed flow rate are summarized.

Table 4.18 Distillate composition response to a -15% step change in feed flow rate.

**DISTILLATE PRODUCT WITH 85% FEED
(N-BUTANE)**

TIME	FULL-ORDER	FIVE (5) COMPARTMENT	FOUR (4) COMPARTMENT
0.0000	0.480140	0.480140	0.480140
0.0011	0.480310	0.475047	0.480140
0.0021	0.480108	0.470607	0.473706
0.0031	0.479717	0.466687	0.468376
0.0041	0.479091	0.462407	0.463900
0.0051	0.478195	0.457839	0.459279
0.0061	0.477213	0.453872	0.454689
0.0071	0.476098	0.450126	0.451019
0.0081	0.474888	0.446645	0.447881
0.0091	0.473564	0.443437	
0.0101	0.472159		
0.0111	0.470703		
0.0121	0.469213		
0.0131	0.467694		
0.0141	0.466156		

Table 4.19 Bottom composition response to a -15% step change in feed flow rate.

**BOTTOM PRODUCT WITH 85% FEED
(N-BUTANE)**

TIME	FULL-ORDER	FIVE (5) COMPARTMENT	FOUR (4) COMPARTMENT
0.0000	0.004760	0.004760	0.004760
0.0011	0.004677	0.004734	0.004748
0.0021	0.004597	0.004705	0.004734
0.0031	0.004548	0.004675	0.004718
0.0041	0.004547	0.004644	0.004699
0.0051	0.004556	0.004615	0.004679
0.0061	0.004536	0.004598	0.004664
0.0071	0.004542	0.004593	0.004655
0.0081	0.004645	0.004605	0.004654
0.0091	0.004746	0.004636	0.004665
0.0101	0.004905	0.004688	0.004687
0.0111	0.005150	0.004757	0.004725
0.0121	0.005456	0.004843	0.004779
0.0131	0.005792	0.004943	
0.0141	0.006172		

4.2.3 Comparison of the intermediate stages

Study of the accuracy of the intermediate stages, comparison of dynamic responses in various stages between a four-compartmental model and a full-order model are summarized in Table 4.20.

Table 4.20 Composition responses of sensitive tray for +15% step change in feed flow rate.

N-BUTANE COMPOSITIONS IN SENSITIVE TRAY

Time	Stage 2		Stage 6		Stage 9		Stage 22	
	Full-Order	Four (4) Compart.	Full-Order	Four (4) Compart.	Full-Order	Four (4) Compart.	Full-Order	Four (4) Compart.
0.0000	0.017270	0.017270	0.083960	0.083960	0.167200	0.167200	0.677840	0.677840
0.0011	0.017013	0.015568	0.083044	0.079617	0.161196	0.162110	0.673998	0.690007
0.0021	0.016677	0.014651	0.082069	0.076813	0.157714	0.160565	0.670399	0.690024
0.0030	0.016399	0.014065	0.081086	0.074874	0.155201	0.159935	0.667487	0.702524
0.0040	0.016051	0.013603	0.079946	0.073250	0.152790	0.159454	0.664733	0.707484
0.0051	0.015745	0.013264	0.078767	0.071976	0.150484	0.158895	0.662258	0.712820
0.0061	0.015507	0.013110	0.077853	0.071261	0.148698	0.158449	0.660517	0.714813
0.0071	0.015324	0.013063	0.077077	0.070878	0.147188	0.158013	0.659276	0.716379
0.0081	0.015180	0.013120	0.076523	0.070796	0.145978	0.157684	0.658615	0.719523
0.0091	0.015169	0.013259	0.076213	0.070946	0.145110	0.157377	0.658656	0.722288
0.0101	0.015253	0.013467	0.076189	0.071297	0.144579	0.157180	0.659368	0.724694
0.0111	0.015446	0.013707	0.076468	0.071757	0.144313	0.156974	0.660683	0.728813
0.0121	0.015725	0.013962	0.077099	0.072268	0.144336	0.156817	0.662572	0.728692
0.0131	0.016180		0.078120		0.144644		0.664934	
0.0141	0.016734		0.079520		0.145213		0.667594	