

	A	B	C	D	E	F	G	H	I	J
1	Styrene Production - Successive Substitution for Recycle Stream									
2										
3		Trigger	0	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000000	iteration count x 10 <sup>-8</sup>						
5										
6		Reaction	C8H10 ----> C8H8 + H2	Conversion		0.65				
7										
8	Iteration #k									
9			(x <sub>n</sub> <sup>k</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k</sup> )
10		Feed	Recycle	Reactor_In	Reactor_Out	Water_Out	Vapor_Out	Organic_Out	Product	New Recycle
11	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.5355777	53.02218822
12	N(C8H8)	0	1.004691135	1.004691135	100.4691135	0	0	100.4691135	99.464422	1.004691135
13	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
14	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
15	N(total)	3100	54.02687935	3154.026879	3253.491302	3000	99.46442234	154.0268794	100	54.02687935
16										
17										
18	Iteration #k+1									
19			(x <sub>n</sub> <sup>k+1</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k+1</sup> )
20		Feed	Recycle	Reactor_In	Reactor_Out	Water_Out	Vapor_Out	Organic_Out	Product	New Recycle
21	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.5355777	53.02218822
22	N(C8H8)	0	1.004691135	1.004691135	100.4691135	0	0	100.4691135	99.464422	1.004691135
23	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
24	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
25	N(total)	3100	54.02687935	3154.026879	3253.491302	3000	99.46442234	154.0268794	100	54.02687935

**FIGURE 3.10**

	A	B	C	D	E	F	G	H	I	J	K	L
1	Start of successive substitution directly on Excel sheet								Name:	Knopf		
2												
3	Recycle and Iteration - Styrene Process								Enter data into outlined cells only			
4	Successive Substitution											
5				Add Needed Recycle								
6				Balances Here			C <sub>8</sub> H <sub>10</sub>	0.35				
7			C <sub>8</sub> H <sub>10</sub>	0.00			C <sub>8</sub> H <sub>8</sub>	64.35				65
8			C <sub>8</sub> H <sub>8</sub>	0.00			Total	64.70		C <sub>8</sub> H <sub>10</sub>	35.00	H <sub>2</sub>
9			Total	0.00						C <sub>8</sub> H <sub>8</sub>	65	
10										Total	100.00	
11							Sep 2					
12	C <sub>8</sub> H <sub>10</sub>	100.00					Reactor					
13												
14	H <sub>2</sub> O	3000.00	C <sub>8</sub> H <sub>10</sub>	100.00					C <sub>8</sub> H <sub>10</sub>	35.00		
15			C <sub>8</sub> H <sub>8</sub>	0.00			C <sub>8</sub> H <sub>10</sub> -> C <sub>8</sub> H <sub>8</sub> + H <sub>2</sub>		C <sub>8</sub> H <sub>8</sub>	65.00		
16			H <sub>2</sub> O	3000.00			Conversion	65%	H <sub>2</sub>	65.00		H <sub>2</sub> O
17			Total	3100.00					H <sub>2</sub> O	3000.00		3000
18									Total	3165.00		
19												
20												
21	Trigger		0	(either 0 to reset or 1 to iterate)								
22	Iterations		0.00000000	iteration count x 10 <sup>-8</sup>								

FIGURE 3.11

	A	B	C	D	E	F	G	H	I	J
1	Styrene Production - Wegstein Method for Recycle Stream									
2										
3		Trigger	0	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000000	iteration count x 10 <sup>-8</sup>						
5		Precision	0.0000001							
6		Reaction	C8H10 ----> C8H8 + H2	Conversion	0.65					
7										
8	Iteration #1		(k=1)							
9			(x <sub>n</sub> <sup>1</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>1</sup> )
10		Feed	Recycle	Reactor_In	Reactor_Out	Water_Out	Vapor_Out	Organic_Out	Product	New Recycle
11	N(C8H10)	100	0	100	35	0	0	35	0.35	34.65
12	N(C8H8)	0	0	0	65	0	0	65	64.35	0.65
13	N(H2)	0	0	0	65	0	65	0	0	0
14	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
15	N(total)	3100	0	3100	3165	3000	65	100	64.7	35.3
16										
17										
18	Iteration #2		(k=2)							
19			(x <sub>n</sub> <sup>2</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>2</sup> )
20		Feed	Recycle	Reactor_In	Reactor_Out	Water_Out	Vapor_Out	Organic_Out	Product	New Recycle
21	N(C8H10)	100	34.65	134.65	47.1275	0	0	47.1275	0.471275	46.656225
22	N(C8H8)	0	0.65	0.65	88.1725	0	0	88.1725	87.290775	0.881725
23	N(H2)	0	0	0	87.5225	0	87.5225	0	0	0
24	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
25	N(total)	3100	35.3	3135.3	3222.8225	3000	87.5225	135.3	87.76205	47.53795
26										
27	Calculate Wegstein parameters - Must solve for every species					Theta max	10			
28						Theta min	-10			
29										
30								(x <sub>n</sub> <sup>3</sup> )		
31			Slope	Theta Calc	Theta Lower	Theta Upper	Wegstein Recycle			
32		N(C8H10)	0.3465	1.530221882	1.530221882	1.530221882	53.02218822			
33		N(C8H8)	0.3565	1.554001554	1.554001554	1.554001554	1.01010101			
34		N(H2)	0	1	1	1	0			
35		N(H2O)	0	1	1	1	0			
36		N(total)								
37										
38										
39	Iteration #3		(k=3)							
40			(x <sub>n</sub> <sup>3</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>3</sup> )
41		Feed	Recycle	Reactor_In	Reactor_Out	Water_Out	Vapor_Out	Organic_Out	Product	New Recycle
42	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.5355777	53.02218822
43	N(C8H8)	0	1.01010101	1.01010101	100.4745234	0	0	100.4745234	99.469778	1.004745234
44	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
45	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
46	N(total)	3100	54.03228923	3154.032289	3253.496712	3000	99.46442234	154.0322892	100.00536	54.02693345

FIGURE 3.13

Option Explicit	line 1
Public Sub Flowsheet_Iteration()	line 2
Dim n_components As Integer	line 3
n_components = 4	
' Dimension x and g values	
Dim x_old() As Double	line 4
ReDim x_old(n_components)	line 5
Dim g_old() As Double	line 6
ReDim g_old(n_components)	line 7
Dim x_current() As Double	line 8
ReDim x_current(n_components)	line 9
Dim g_current() As Double	line 10
ReDim g_current(n_components)	line 11
' Call Successive Substitution for first two iterations	
Call Successive(x_old, g_old, x_current, g_current, n_components)	line 12
' Call Wegstein Method	
Call Wegstein(x_old, g_old, x_current, g_current, n_components)	line 13
End Sub	line 14
Sub Successive(x_old, g_old, x_current, g_current, n_components)	line 15
' Read x1 and resulting g(x1) values from sheet	
Dim i As Integer	line 16
For i = 0 To n_components - 1	line 17
x_old(i) = Sheet1.Cells(i + 11, 3)	line 18
g_old(i) = Sheet1.Cells(i + 11, 10)	line 19
Next i	line 20
' Place g(x1) values on sheet as new x2 values	
For i = 0 To n_components - 1	line 21
Sheet1.Cells(i + 11, 3) = g_old(i)	line 22
Next i	line 23
' Read x2 and resulting g(x2) values from sheet	
For i = 0 To n_components - 1	line 24
x_current(i) = Sheet1.Cells(i + 11, 3)	line 25
g_current(i) = Sheet1.Cells(i + 11, 10)	line 26
Next i	line 27
End Sub	line 28
Sub Wegstein(x_old, g_old, x_current, g_current, n_components)	line 29
Dim Slope() As Double	line 30
ReDim Slope(n_components)	line 31
Dim Theta() As Double	line 32
ReDim Theta(n_components)	line 33

**FIGURE 3.15a**

```

Dim x_new() As Double                                line 34
ReDim x_new(n_components)                            line 35

' Set up Wegstein Method iteration loop using j as counter

Dim j As Integer                                    line 36
Dim i As Integer                                    line 37

Dim Max_Iteration As Integer                          line 38
Max_Iteration = 10                                   line 39
For j = 1 To Max_Iteration                           line 40

    ' Then calculate Slope and Theta
    For i = 0 To n_components - 1                    line 41
        If (x_current(i) - x_old(i) = 0.0#) Then      line 42
            Slope(i) = 0.0#                           line 43
        Else                                           line 44
            Slope(i) = (g_current(i) - g_old(i)) / (x_current(i) - x_old(i))
                                                         line 45
        End If                                         line 46

        If ((1 - Slope(i)) = 0.0#) Then                line 47
            Theta(i) = 1                               line 48
        Else                                           line 49
            Theta(i) = 1 / (1 - Slope(i))              line 50
        End If                                         line 51

        ' Check extrapolation bounds
        If Theta(i) >= 10.0# Then Theta(i) = 10.0#     line 52
        If Theta(i) <= -10.0# Then Theta(i) = -10.0#   line 53

        ' Calculate new x values for sheet
        x_new(i) = (1.0# - Theta(i)) * x_current(i) + Theta(i) * g_current(i)
                                                         line 54
    Next i                                             line 55

    ' Place new x values on sheet

    For i = 0 To n_components - 1                    line 56
        Sheet1.Cells(i + 11, 3) = x_new(i)            line 57
    Next i                                             line 58

    ' Set x and g values
    For i = 0 To n_components - 1                    line 59
        x_old(i) = x_current(i)                      line 60
        g_old(i) = g_current(i)                      line 61
        x_current(i) = Sheet1.Cells(i + 11, 3)        line 62
        g_current(i) = Sheet1.Cells(i + 11, 10)        line 63
    Next i                                             line 64

    ' Here we could check a convergence criterion parameter
    ' (Max_Change) to allow code exit or
    ' Continue to loop until Max_Iterations

Next j                                                line 65
End Sub                                              line 66

```

**FIGURE 3.15b**

	A	B	C	D	E	F	G	H	I	J
1	<b>Styrene Production Alternative Specification - Trial and Error Solution</b>									
2										
3		Trigger	0	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000000	iteration count x 10 <sup>-8</sup>						
5										
6		Reaction	C8H10 ----> C8H8 + H2		Conversion	0.65				
7										
8	<b>Iteration #k</b>	to start set Recycle column = 0, then set Recycle = k+1 New Recycle Column								
9			(x <sub>n</sub> <sup>k</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k</sup> )
10		<b>Feed</b>	<b>Recycle</b>	<b>Reactor In</b>	<b>Reactor Out</b>	<b>Water Out</b>	<b>Vapor Out</b>	<b>Organic Out</b>	<b>Product</b>	<b>New Recycle</b>
11	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.5355777	53.02218822
12	N(C8H8)	0	1.004691135	1.004691135	100.4691135	0	0	100.4691135	99.464422	1.004691135
13	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
14	N(H2O)	0	0	0	0	0	0	0	0	0
15	N(total)	100	54.02687935	154.0268794	253.4913017	0	99.46442234	154.0268794	100	54.02687935
16			water mol fraction	0						
17										
18	<b>Iteration #k+1</b>									
19			(x <sub>n</sub> <sup>k+1</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k+1</sup> )
20		<b>Feed</b>	<b>Recycle</b>	<b>Reactor In</b>	<b>Reactor Out</b>	<b>Water Out</b>	<b>Vapor Out</b>	<b>Organic Out</b>	<b>Product</b>	<b>New Recycle</b>
21	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.5355777	53.02218822
22	N(C8H8)	0	1.004691135	1.004691135	100.4691135	0	0	100.4691135	99.464422	1.004691135
23	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
24	N(H2O)	0	0	0	0	0	0	0	0	0
25	N(total)	100	54.02687935	154.0268794	253.4913017	0	99.46442234	154.0268794	100	54.02687935

**FIGURE 3.17**

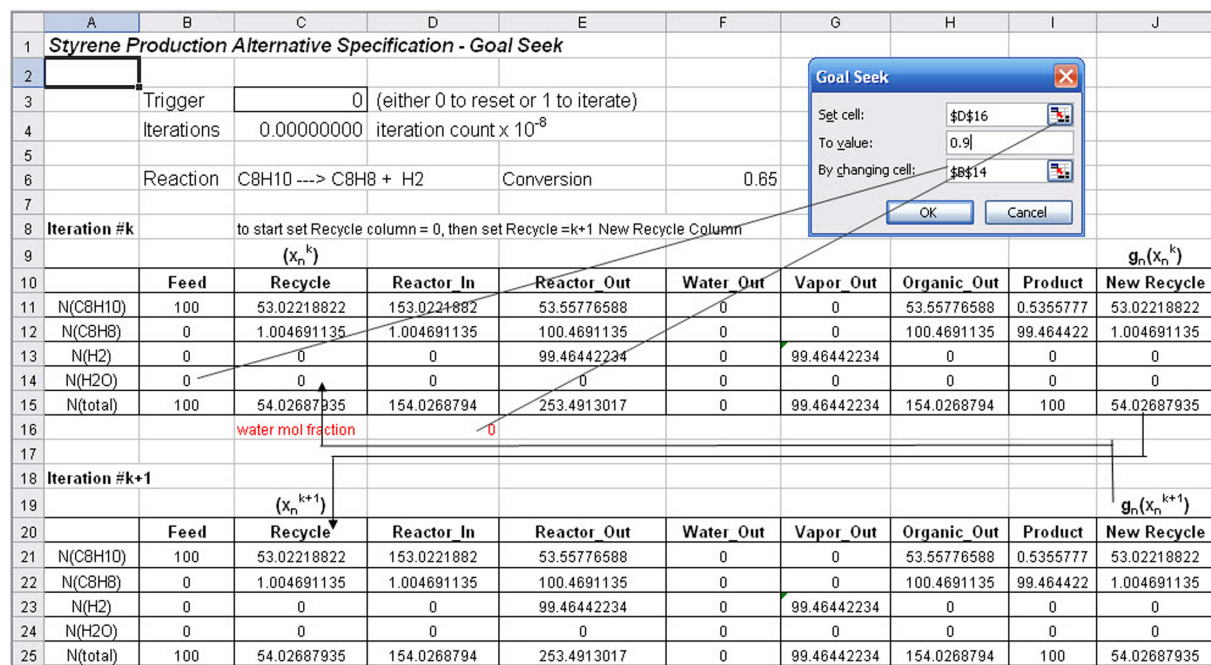


FIGURE 3.18

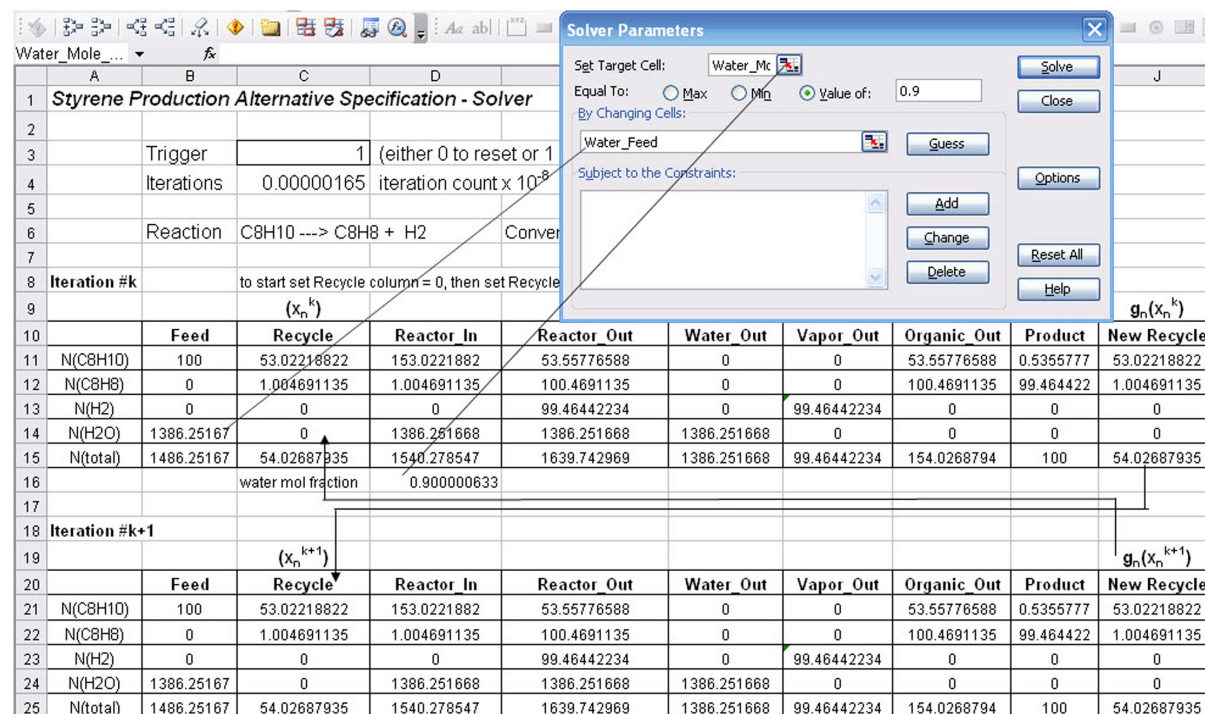


FIGURE 3.19

	A	B	C	D	E	F	G	H	I	J
1	<b>Styrene Production Wegstein Method / VBA / WB Solver</b>									
2										
3		Trigger	1	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000097	iteration count x 10 <sup>-8</sup>						
5										
6		Reaction	C8H10 ----> C8H8 + H2	Conversion	0.65					
7										
8	<b>Iteration</b>									
9			(x <sub>n</sub> )							g <sub>n</sub> (x <sub>n</sub> )
10		<b>Feed</b>	<b>Recycle</b>	<b>Reactor_In</b>	<b>Reactor_Out</b>	<b>Water_Out</b>	<b>Vapor_Out</b>	<b>Organic_Ou</b>	<b>Product</b>	<b>New Recycle</b>
11	N(C8H10)	100	53.02218822	153.022188	53.55776588	0	0	53.557766	0.535577659	53.02218822
12	N(C8H8)	0	1.004691135	1.00469113	100.4691135	0	0	100.46911	99.46442234	1.004691135
13	N(H2)	0	0	0	99.46442234	0	99.4644223	0	0	0
14	N(H2O)	1377.0512	0	1377.05116	1377.05116	1377.05116	0	0	0	0
15	N(total)	1477.0512	54.02687935	1531.07804	1630.542462	1377.05116	99.4644223	154.02688	100	54.02687935
16				0.89939972	H <sub>2</sub> O mole fraction					
17				3.6034E-07	Objective Function					

**FIGURE 3.20**

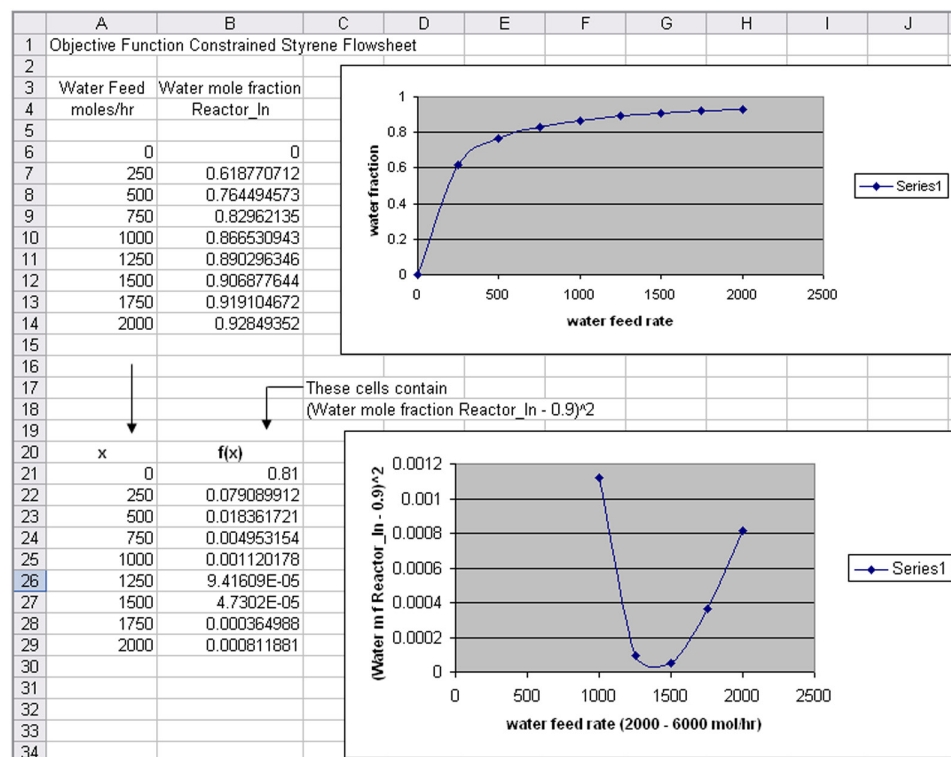
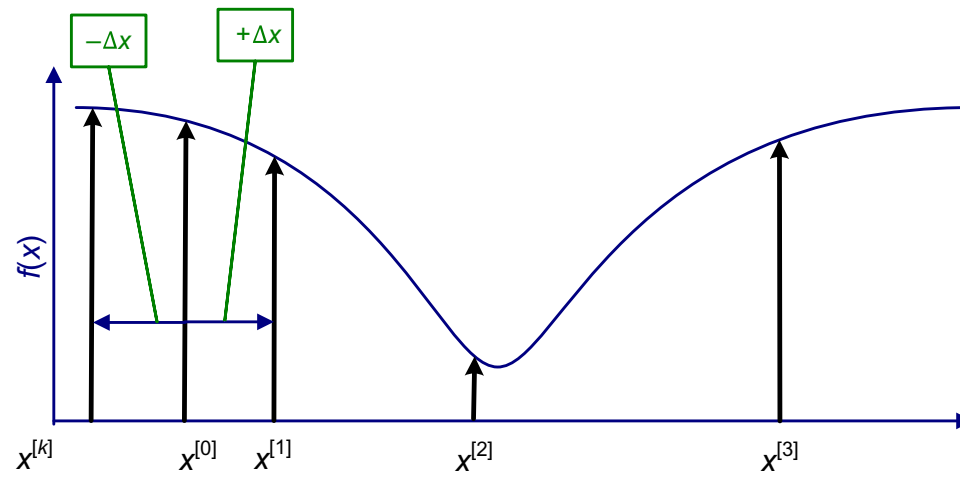


FIGURE 3.21



**FIGURE 3.22**

	A	B	C	D	E	F	G	H	I	J	K	L
1	Styrene Flowsheet with constraint - VBA Bounding Phase									Name:	Knopf	
2						$x^0 =$	200		Enter data into red cells only			
3						$\Delta x =$	50		$x^{\text{left}} =$	950.00	Min Steam (H <sub>2</sub> O)	
4									$x^{\text{right}} =$	3350.00	Max Steam (H <sub>2</sub> O)	
5									Needed	0.9	(mol H <sub>2</sub> O/mol total)	
6							C <sub>8</sub> H <sub>10</sub>	0.54				
7			C <sub>8</sub> H <sub>10</sub>	53.0222			C <sub>8</sub> H <sub>8</sub>	99.46442		C <sub>8</sub> H <sub>10</sub>	53.5578	99.46
8			C <sub>8</sub> H <sub>8</sub>	1.0047			Total	100.00		C <sub>8</sub> H <sub>8</sub>	100.4691	H <sub>2</sub>
9			Total	54.0269						Total	154.0269	
10						Sep 2						
11												
12	C <sub>8</sub> H <sub>10</sub>	100.00				Reactor						
13												
14	H <sub>2</sub> O	3350.00	C <sub>8</sub> H <sub>10</sub>	153.02			C <sub>8</sub> H <sub>10</sub> → C <sub>8</sub> H <sub>8</sub> + H <sub>2</sub>		C <sub>8</sub> H <sub>10</sub>	53.56		
15			C <sub>8</sub> H <sub>8</sub>	1.00			Conversion	65%	C <sub>8</sub> H <sub>8</sub>	100.47		
16			H <sub>2</sub> O	3350.00					H <sub>2</sub>	99.46		
17			Total	3504.03					H <sub>2</sub> O	3350.00	3350	
18									Total	3603.49		
19												
20												
21			Steam mol frac	0.9560429								

FIGURE 3.23

```

Sub Bound()
    ' We want to bound the water feed rate between [xa, xb] or [xleft, xright]
    ' We get the initial guess, x0 now called x1, from cell G2 on the flowsheet

    x1 = Range("G2").Value
    ' We next calculate our objective function
    ' This is done on the flowsheet in a separate Sub Procedure
    Call Flowsheet(x1, F)
    f1 = F

    ' Next we determine the direction for the step delta_x

    delta_x = Range("G3").Value

    xright = x1 + delta_x
    Call Flowsheet(xright, F)
    fright = F
    xleft = x1 - delta_x
    Call Flowsheet(xleft, F)
    fleft = F

    Iteration_limit = 10000
    Iteration = 0
    Do
        If fleft > f1 And fright > f1 Then Exit Do

        If f1 > fright Then
            Iteration = Iteration + 1
            xleft = x1
            fleft = f1
            x1 = xright
            f1 = fright
            xright = x1 + (2 ^ Iteration) * delta_x
            Call Flowsheet(xright, F)
            fright = F

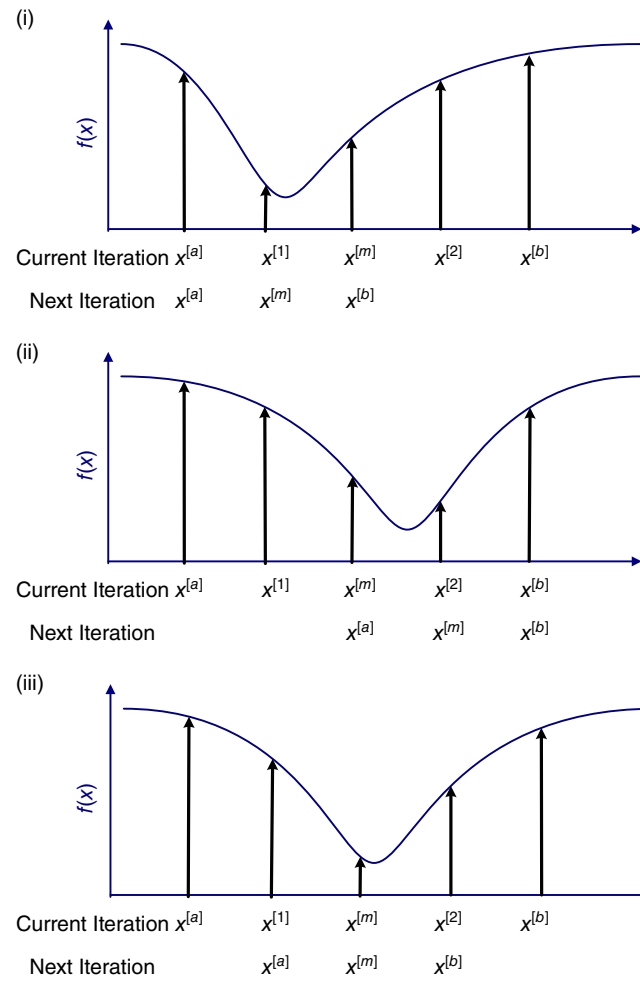
        Else
            Iteration = Iteration + 1
            xright = x1
            fright = f1
            x1 = xleft
            f1 = fleft
            xleft = x1 - (2 ^ Iteration) * delta_x
            ' Normally the next two statements (currently comments) would not
            ' be used as the flow rate can not be negative
            ' If xleft < 0 Then xleft = 0
            ' If xleft = 0 Then Exit Do
            Call Flowsheet(xleft, F)
            fleft = F

        End If
    Loop Until Iteration > Iteration_limit
    ' Place bounded water flow on spreadsheet as [xa, xb] or [xleft, xright]
    Range("J3").Value = xleft
    Range("J4").Value = xright
End Sub

Sub Flowsheet(x, F)
    ' Here we place the water flow rate on the flowsheet in cell B14
    ' the flowsheet will converge before it returns control to the VBA code.
    Range("B14").Value = x
    ' The flowsheet is now converged with the x value (water flow rate)
    ' Cell D21 contains the converged (moles H2O)/(Total moles in Reator)
    ' Cell J5 contains the desired (moles H2O)/(Total moles in Reator)
    ' We square the difference between converged and desired (mole fraction)
    F = (Range("D21").Value - Range("J5").Value) ^ 2
    ' The value in F will be returned to the Bounding Sub Procedure
End Sub

```

**FIGURE 3.24**



**FIGURE 3.25**

	A	B	C	D	E	F	G	H	I	J	K	L
1	Styrene Flowsheet Interval Halving								Name:	Knopf		
2									Enter data into red cells only			
3	Enter Bounding Results in Red Cells								$x^{\text{left}} =$	950.00	Min Steam (H <sub>2</sub> O)	
4									$x^{\text{right}} =$	3350.00	Max Steam (H <sub>2</sub> O)	
5									Needed	0.9	(mol H <sub>2</sub> O/mol total)	
6							C <sub>8</sub> H <sub>10</sub>	0.54				
7			C <sub>8</sub> H <sub>10</sub>	53.0222			C <sub>8</sub> H <sub>8</sub>	99.46442				99.46
8			C <sub>8</sub> H <sub>8</sub>	1.0047			Total	100.00		C <sub>8</sub> H <sub>10</sub>	53.5578	H <sub>2</sub>
9			Total	54.0269						C <sub>8</sub> H <sub>8</sub>	100.4691	
10										Total	154.0269	
11						Sep 2						
12	C <sub>8</sub> H <sub>10</sub>	100.00				Reactor						
13												
14	H <sub>2</sub> O	1386.24	C <sub>8</sub> H <sub>10</sub>	153.02					C <sub>8</sub> H <sub>10</sub>	53.56		
15			C <sub>8</sub> H <sub>8</sub>	1.00			C <sub>8</sub> H <sub>10</sub> → C <sub>8</sub> H <sub>8</sub> + H <sub>2</sub>		C <sub>8</sub> H <sub>8</sub>	100.47		
16			H <sub>2</sub> O	1386.24		Conversion	65%		H <sub>2</sub>	99.46		H <sub>2</sub> O
17			Total	1540.27					H <sub>2</sub> O	1386.24		1386.24
18									Total	1639.73		
19												
20												
21			Steam mol frac	0.9								
22												
23												
24	Trigger	0	(either 0 to reset or 1 to iterate)									
25	Iterations	0.00000000	iteration count x 10 <sup>-8</sup>									

FIGURE 3.26

```

Sub Interval_Halving()
    ' We specify that our function has been bounded
    ' between [xa, xb] or [xleft, xright]
    ' and here xa and xb are given on the flowsheet (in cells J3 and J4,
    respectively)
    '
    ' We get the lower bound, xa, from cell J3 on the flowsheet
    ' here xa is our lower bound on the water (steam) flow rate
    xa = Range("J3").Value
    ' Here we call our "function" - which is generally done in a separate Sub
    Procedure
    Call Flowsheet(xa, F)
    fa = F
    ' Here we get the upper bound, xb, from cell J4 on the flowsheet
    xb = Range("J4").Value
    Call Flowsheet(xb, F)
    fb = F
    ' Here we determine the mid point
    xm = (xa + xb) / 2
    Call Flowsheet(xm, F)
    fm = F
    Max_Change = 0.000001
    Iteration_limit = 100000
    Iteration = 0
    Do
        Iteration = Iteration + 1
        delta_x = (xb - xa)
        If Abs(xb - xa) < Max_Change Then Exit Do
        ' Here we determine the points 1/4 and 3/4 of the total length
        x1 = xa + delta_x / 4
        Call Flowsheet(x1, F)
        f1 = F
        x2 = xb - delta_x / 4
        Call Flowsheet(x2, F)
        f2 = F
        If f1 < fm Then
            xa = xa
            xb = xm
            xm = x1
            fm = f1
        ElseIf f2 < fm Then
            xb = xb
            xa = xm
            xm = x2
            fm = f2
        Else
            xa = x1
            xb = x2
            xm = xm
            fm = fm
        End If
    Loop Until Iteration > Iteration_limit
    ' Here the optimum, xm, will be placed in the spreadsheet
    ' and one last convergence performed
    Range("B14").Value = xm
End Sub

Sub Flowsheet(x, F)
    ' Here we place the water flow rate on the flowsheet in cell B14
    ' the flowsheet will converge before it returns control to the VBA code.
    Range("B14").Value = x
    ' The flowsheet is now converged with the x value (water flow rate)
    ' Cell D21 contains the converged (moles H2O)/(Total moles in Reator)
    ' Cell J5 contains the desired (moles H2O)/(Total moles in Reator)
    ' We square the difference between converged and desired (mole fraction)
    F = (Range("D21").Value - Range("J5").Value) ^ 2
    ' F will be returned to the Interval Halving Sub Procedure
End Sub

```

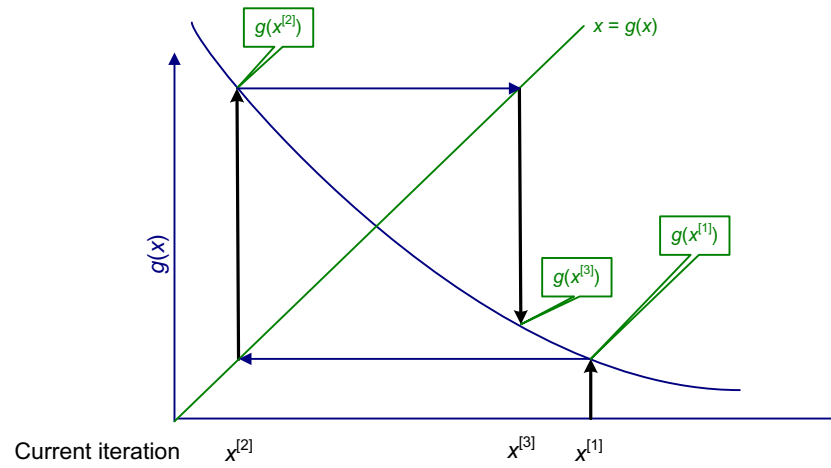
**FIGURE 3.27**

	A	B	C	D	E	F	G	H	I	J
1	<b>Styrene Production Nonlinear Specification - Problem Start</b>									
2										
3		Trigger	0	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000000	iteration count x 10 <sup>-8</sup>						
5										
6		Reaction	C8H10 ----> C8H8 + H2	Conversion	0.65					
7										
8	<b>Iteration #1</b>		(k=1)							
9			(x <sub>n</sub> <sup>1</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>1</sup> )
10		<b>Feed</b>	<b>Recycle</b>	<b>Reactor_In</b>	<b>Reactor_Out</b>	<b>Water_Out</b>	<b>Vapor_Out</b>	<b>Organic_Out</b>	<b>Product</b>	<b>New Recycle</b>
11	N(C8H10)	100	0	100	35	0	0	35	0.35	34.65
12	N(C8H8)	0	0	0	65	0	0	65	64.812884	0.187115573
13	N(H2)	0	0	0	65	0	65	0	0	0
14	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
15	N(total)	3100	0	3100	3165	3000	65	100	65.162884	34.83711557
16										
17										
18	<b>Iteration #2</b>		(k=2)							
19			(x <sub>n</sub> <sup>2</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>2</sup> )
20		<b>Feed</b>	<b>Recycle</b>	<b>Reactor_In</b>	<b>Reactor_Out</b>	<b>Water_Out</b>	<b>Vapor_Out</b>	<b>Organic_Out</b>	<b>Product</b>	<b>New Recycle</b>
21	N(C8H10)	100	34.65	134.65	47.1275	0	0	47.1275	0.471275	46.656225
22	N(C8H8)	0	0.187115573	0.187115573	87.70961557	0	0	87.70961557	87.458205	0.251410516
23	N(H2)	0	0	0	87.5225	0	87.5225	0	0	0
24	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
25	N(total)	3100	34.83711557	3134.837116	3222.359616	3000	87.5225	134.8371156	87.92948	46.90763552

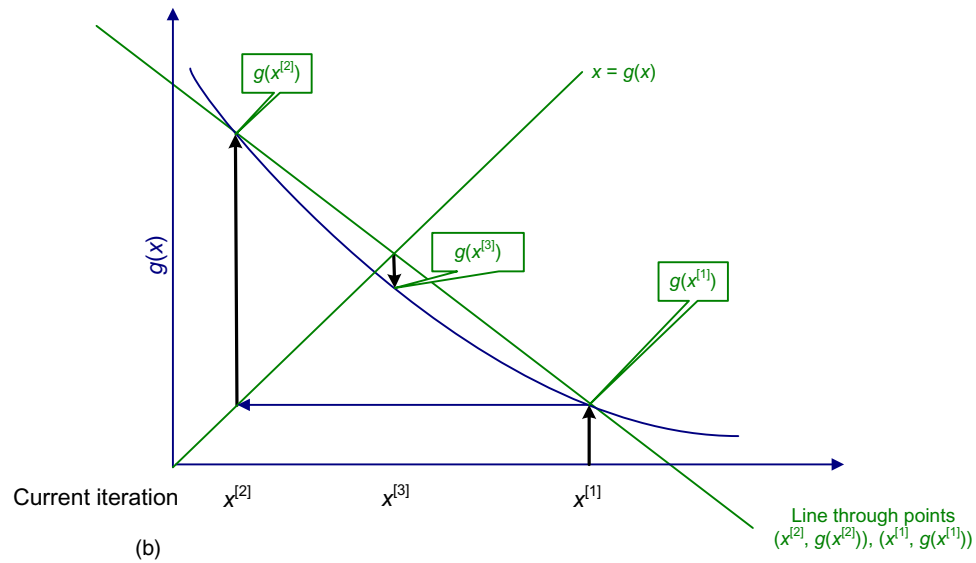
**FIGURE 3.28**

	A	B	C	D	E	F	G	H	I	J
1	<b>Styrene Production Nonlinear Specification</b>									
2										
3		Trigger	0	(either 0 to reset or 1 to iterate)						
4		Iterations	0.00000000	iteration count x 10 <sup>-8</sup>						
5										
6		Reaction	C8H10 ----> C8H8 + H2	Conversion	0.65	mol fraction C <sub>8</sub> H <sub>8</sub> product			0.99464422	
7										
8	Iteration #k						mol fraction C <sub>8</sub> H <sub>10</sub> recycle			0.99464422
9			(x <sub>n</sub> <sup>k</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k</sup> )
10		Feed	Recycle	Reactor In	Reactor Out	Water Out	Vapor Out	Organic Out	Product	New Recycle
11	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.53557766	53.02218822
12	N(C8H8)	0	0.28550409	0.28550409	99.74992643	0	0	99.74992643	99.4644223	0.28550409
13	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
14	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
15	N(total)	3100	53.30769231	3153.307692	3252.772115	3000	99.46442234	153.3076923	100	53.30769231
16										
17										
18	Iteration #k+1									
19			(x <sub>n</sub> <sup>k+1</sup> )							g <sub>n</sub> (x <sub>n</sub> <sup>k+1</sup> )
20		Feed	Recycle	Reactor In	Reactor Out	Water Out	Vapor Out	Organic Out	Product	New Recycle
21	N(C8H10)	100	53.02218822	153.0221882	53.55776588	0	0	53.55776588	0.53557766	53.02218822
22	N(C8H8)	0	0.28550409	0.28550409	99.74992643	0	0	99.74992643	99.4644223	0.28550409
23	N(H2)	0	0	0	99.46442234	0	99.46442234	0	0	0
24	N(H2O)	3000	0	3000	3000	3000	0	0	0	0
25	N(total)	3100	53.30769231	3153.307692	3252.772115	3000	99.46442234	153.3076923	100	53.30769231

**FIGURE 3.29**

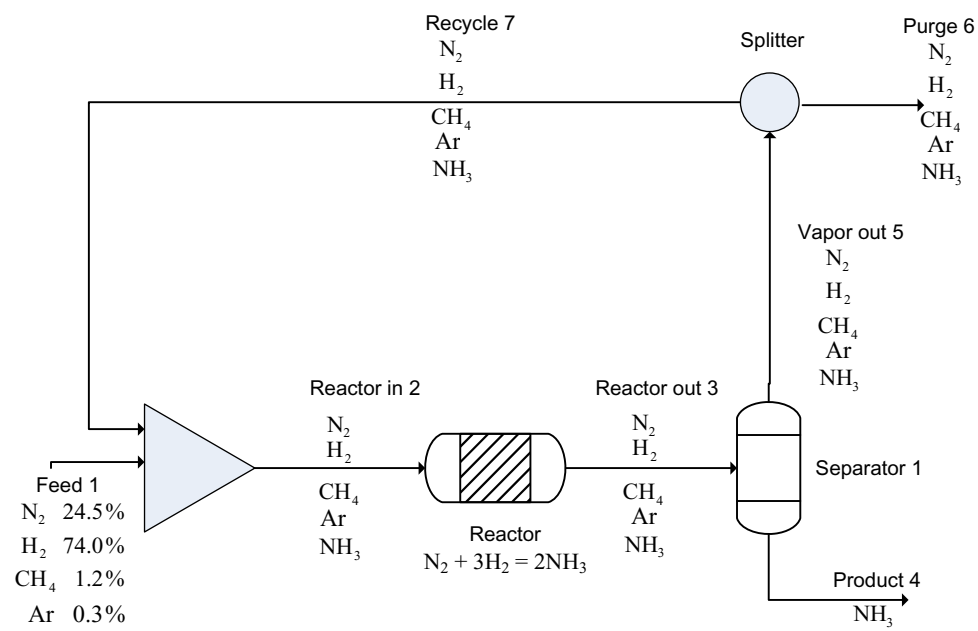


(a)

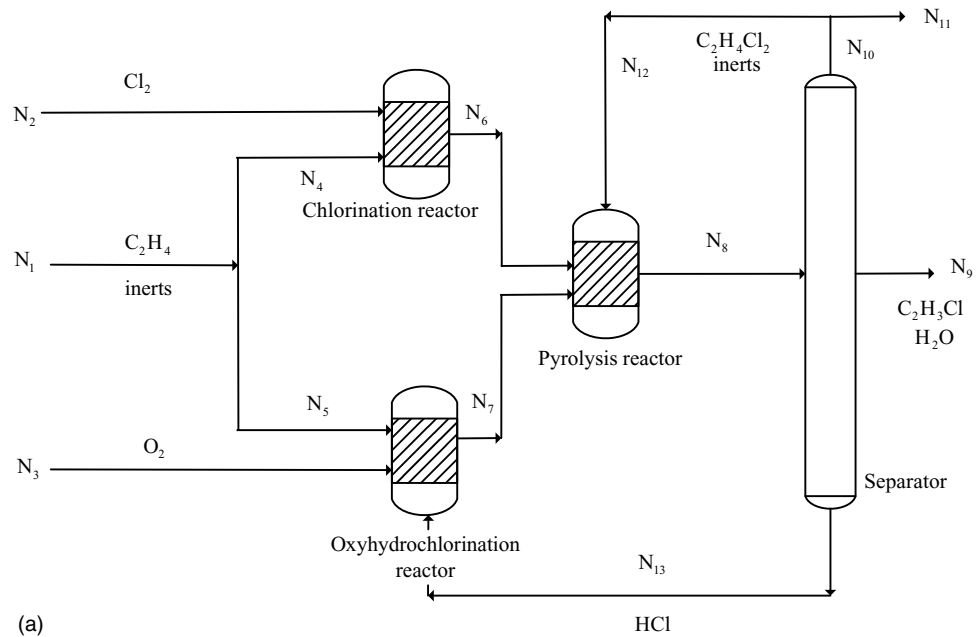


(b)

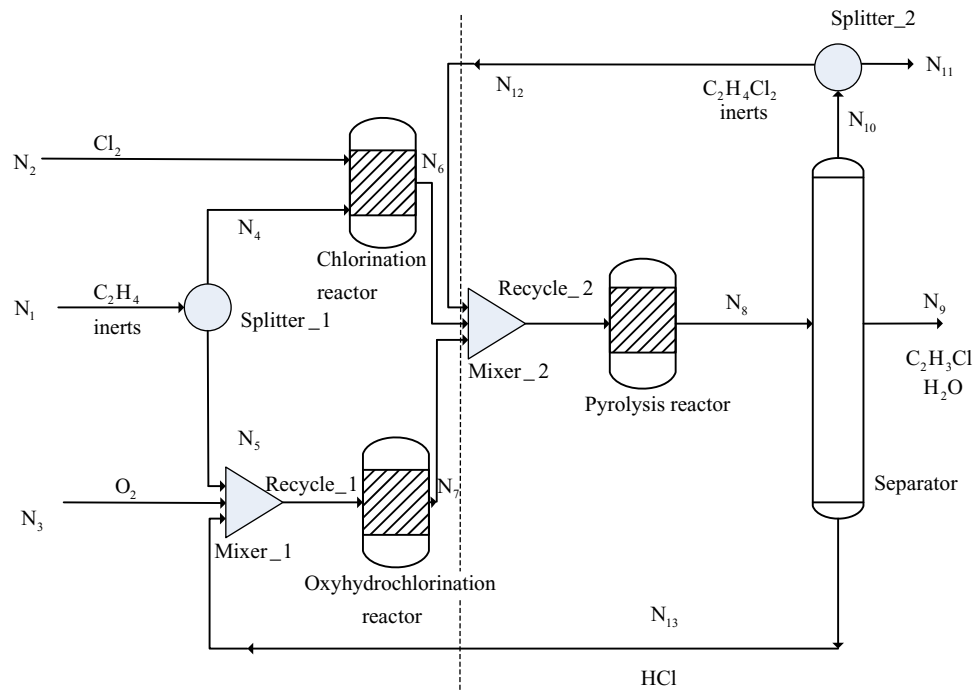
**FIGURE 3.8**



**FIGURE p3.15**

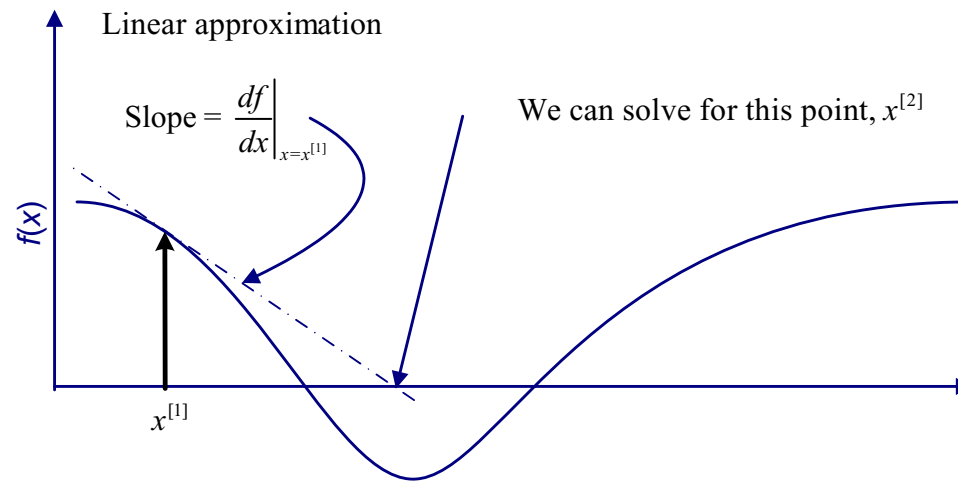


(a)



(b)

FIGURE p3.20



**FIGURE p3.4**