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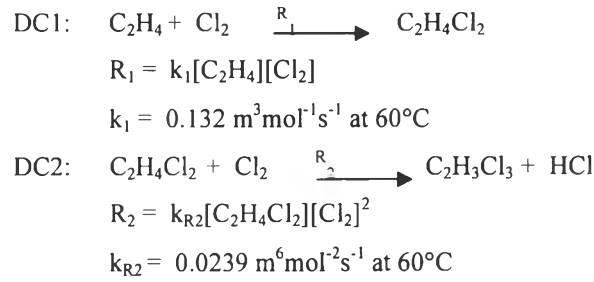
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## APPENDICES

### Appendix A Reactor modeling procedure.

#### Direct Chlorination Reactor Model:

Direct chlorination reaction kinetics were derived from Wachi and Morikawa, 1986. A CSTR reactor was modeled to determine consumption of reactants and production of products.



$$[\text{C}_2\text{H}_4] - [\text{C}_2\text{H}_4]_0 = -k_1[\text{C}_2\text{H}_4][\text{Cl}_2]\tau$$

$$\Rightarrow [\text{C}_2\text{H}_4] = \frac{[\text{C}_2\text{H}_4]_0}{1 + k_1\tau[\text{Cl}_2]}$$

$$[\text{Cl}_2] - [\text{Cl}_2]_0 = -k_1\tau[\text{C}_2\text{H}_4][\text{Cl}_2] - k_2\tau[\text{C}_2\text{H}_4][\text{Cl}_2]^2$$

$$\Rightarrow [\text{Cl}_2] - [\text{Cl}_2]_0 = \frac{-k_1\tau[\text{C}_2\text{H}_4]_0[\text{Cl}_2] - k_2\tau[\text{C}_2\text{H}_4]_0[\text{Cl}_2]^2}{1 + k_1\tau[\text{Cl}_2]}$$

$$\Rightarrow [\text{Cl}_2] - [\text{Cl}_2]_0 + k_1\tau[\text{Cl}_2]^2 - k_1\tau[\text{Cl}_2][\text{Cl}_2]_0 = -k_1\tau[\text{C}_2\text{H}_4]_0[\text{Cl}_2] - k_2\tau[\text{C}_2\text{H}_4]_0[\text{Cl}_2]^2$$

$$\Rightarrow (k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0)[\text{Cl}_2]^2 + (1 + k_1\tau[\text{C}_2\text{H}_4]_0 - k_1\tau[\text{Cl}_2]_0)[\text{Cl}_2] - [\text{Cl}_2]_0 = 0$$

$$\Rightarrow [\text{Cl}_2]^2 + \frac{1 + k_1\tau[\text{C}_2\text{H}_4]_0 - k_1\tau[\text{Cl}_2]_0}{k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0}[\text{Cl}_2] - \frac{1}{k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0}[\text{Cl}_2]_0 = 0$$

$$\Rightarrow [\text{Cl}_2] = \frac{\frac{1 + k_1\tau[\text{C}_2\text{H}_4]_0 - k_1\tau[\text{Cl}_2]_0}{k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0} + \sqrt{\left(\frac{1 + k_1\tau[\text{C}_2\text{H}_4]_0 - k_1\tau[\text{Cl}_2]_0}{k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0}\right)^2 + \frac{4[\text{Cl}_2]_0}{k_1\tau + k_2\tau[\text{C}_2\text{H}_4]_0}}}{2}$$

$$[EDC] - [EDC]_0 = (k_1[C_2H_4][Cl_2] - k_2[C_2H_4][Cl_2]^2)\tau$$

$$\Rightarrow [EDC] = (k_1[C_2H_4][Cl_2] - k_2[C_2H_4][Cl_2]^2)\tau$$

$$[TCE] = [HCl] = k_2[C_2H_4][Cl_2]^2\tau$$

#### Direct Chlorination Reactor Parameters

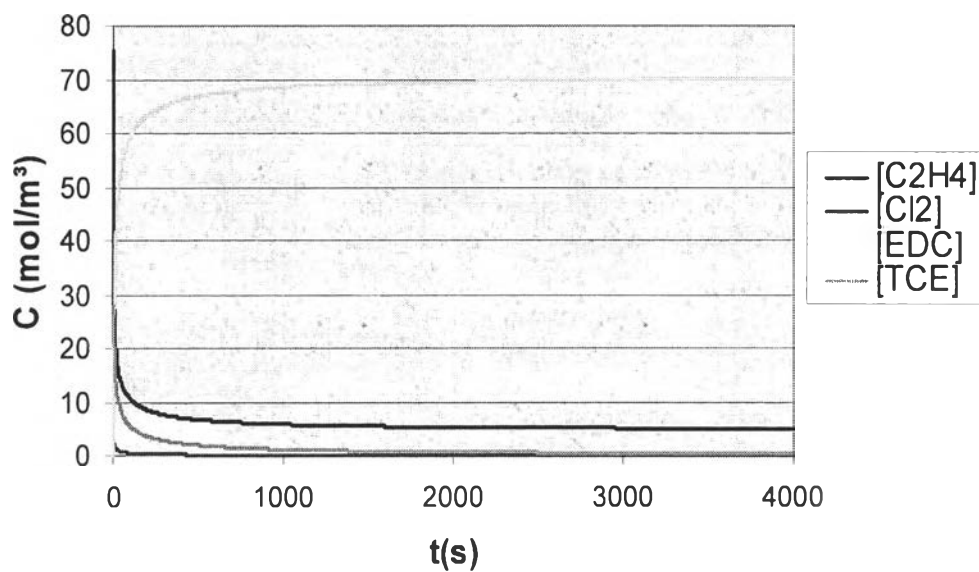
- Residence time = 4000 s
- Pressure = 1 atm
- Temperature = 60 °C

The conversion of  $Cl_2$  = 100%

The selectivity of EDC = 99%

The molar volume in the gas phase ( $V_m$ ) = 146.4 mol/m<sup>3</sup>

#### Direct chlorination of ethylene



#### Fraction of feed components

- $C_2H_2$  = 0.5155
- $Cl_2$  = 0.4845

#### Fraction of effluent components

- $C_2H_2$  = 6.5508E-02
- $Cl_2$  = 3.5425E-04
- EDC = 9.2509E-01
- TCE = 4.5238E-03

- HCl = 4.5238E-03

### Oxy-chlorination Reactor Model:

Oxy-chlorination reaction kinetics was derived from Sai Prasad *et al*, 2001. EDC is formed through a heterogeneous catalytic, cupric chloride catalyst impregnated on a porous alumina support, in PFR. Table A-1 shows the oxy-chlorination reactions.

**Table A1** The oxy-chlorination reactions

Set no.	Reaction	Stoichiometry	Rate of reaction	Frequency factor ( $A_i$ ) (kmol/kg of supp*s*MPa)	Activation energy ( $E_i$ ) (kJ/mol)
R-1	DCE formation	$C_2H_4 + 2CuCl_2 \rightarrow C_2H_4Cl_2 + 2CuCl$	$r_1 = k_1 \rho_s p^{(1)} S^{(1)}$	1.849E8	97.72E3
R-2	TCE formation	$C_2H_4 + 3CuCl_2 \rightarrow C_2H_3Cl_3 + 3CuCl + \frac{1}{2}H_2$	$r_2 = k_2 \rho_s p^{(1)} S^{(1)}$	1.672E8	111.30E3
R-3	$C_2H_4$ combustion	$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$	$r_3 = k_3 p^{(1)} p^{(2)}$	7.759E1	129.7E3
R-4	CuCl oxidation	$2CuCl + \frac{1}{2}O_2 \rightarrow CuO-CuCl_2 \rightarrow CuO + CuCl_2$	$r_4 = k_4 \rho_s p^{(2)} S^{(2)}$	3.446E8	86.97E3
R-5	$CuCl_2$ regeneration	$CuO + 2HCl \rightarrow CuCl_2 + H_2O$	$r_5 = k_5 \rho_s p^{(3)} S^{(3)}$	8.329E13	144.3E3
R-6	$CuCl_2$ evaporation	$CuCl_2$ (solid) $\rightarrow$ $CuCl_2$ (vapor)	$r_6 = k_6 \rho_s$	9.95E3	65.00E3
R-7	$CuCl_2$ condensation	$CuCl_2$ (vapor) $\rightarrow$ $CuCl_2$ (solid)	$r_7 = k_7 \rho_s$	9.546	65.00E3

Where  $k_j = A_j \exp(-E/RT)$

$k_j$  = rate of reaction  $i$  (kmol/m<sup>3</sup>\*s)

$\rho_s$  = bulk density of the catalyst support (kg/m<sup>3</sup>)

$S^{(i)}$  = concentration of solid species (kmol/kg of the support)

$p^{(i)}$  = partial pressure of species  $i$  (MPa)

A plug flow reactor molar continuity equation was introduced to determine consumption of reactants and production of products.

$$\frac{dF_k}{dz} = v r_i A_t \Rightarrow dF_k = v r_i A_t dz$$

where :  $F_k$  = molar flow rate  $k$   
 $z$  = tube length  
 $A_t$  = tube section  
 $r_i$  = reaction rate constant  $i$

From the molar continuity equation,  $dF_k$  was derived

$$\text{Ethylene : } dF_E = A_t dz \cdot (-k_1 \rho_s p^E s^{\text{CuCl}_2} - k_2 \rho_s p^E s^{\text{CuCl}_2} - k_3 \rho^E p^{O_2})$$

$$\text{Oxygen : } dF_O = A_t dz \cdot (-3k_3 p^E p^O - \frac{1}{2} k_4 \rho_s p^O s^{\text{CuCl}})$$

$$\text{HCl : } dF_H = A_t dz \cdot (-2k_5 \rho_s p^H s^{\text{CuO}})$$

$$\text{EDC : } dF_{\text{EDC}} = A_t dz \cdot (k_1 \rho_s p^E s^{\text{CuCl}_2})$$

$$\text{TEC : } dF_T = A_t dz \cdot (k_2 \rho_s p^E s^{\text{CuCl}_2})$$

$$\text{Water : } dF_W = A_t dz \cdot (2k_3 p^E p^O + k_5 \rho_s p^H s^{\text{CuO}})$$

$$\text{CO}_2 : dF_C = A_t dz \cdot (2k_3 p^E p^O)$$

$$\text{CuCl}_2 : dF_{\text{CuCl}_2} = A_t dz \cdot (k_6 \rho_s - k_7 \rho_s)$$

$$[\text{CuCl}_2]_s = [\text{HCl}] \cdot 0.886$$

$$[\text{CuO}] = \frac{k_4 p^O [\text{CuCl}]}{k_5 [p^H]}$$

$$[\text{CuCl}] = \frac{p^E [\text{CuCl}_2] [2k_1 + 3k_2]}{2k_4 p^O}$$

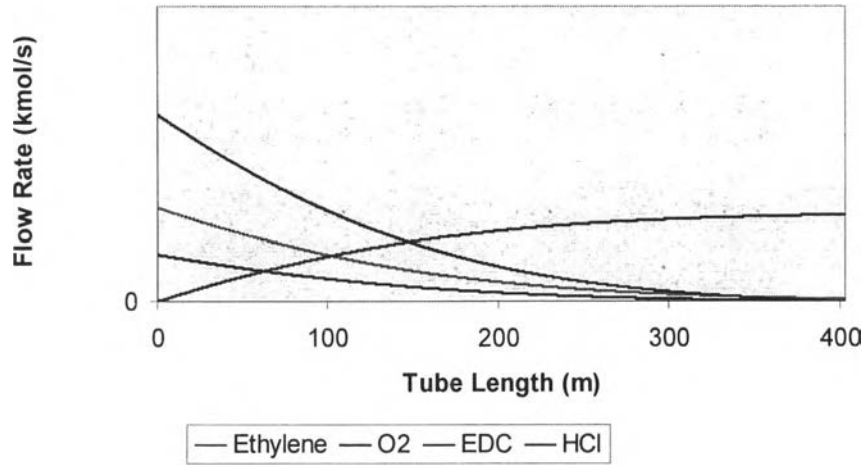
#### Oxy-chlorination Reactor Parameters

- Tube diameter = 30 cm
- Tube length = 400 m
- Pressure = 0.5 MPa
- Temperature = 310 °C
- $[\text{CuCl}_2]$  =  $[\text{HCl}] \cdot 0.886$  kmol/m<sup>3</sup>

The conversion of ethylene = 46.8%

The selectivity of EDC = 97.4%

### Oxychlorination Reactor



#### Fraction of feed components

- $C_2H_2 = 0.2857$
- $HCl = 0.5714$
- $Oxygen = 0.1429$

#### Fraction of effluent components

- $C_2H_2 = 1.2812E-02$
- $O_2 = 6.4746E-05$
- $HCl = 2.5898E-04$
- $EDC = 4.6173E-01$
- $TCE = 2.5365E-02$
- $Water = 4.9977E-01$
- $CO_2 = 1.0038E-10$

#### Pyrolysis Reactor Model:

Vinyl chloride monomer is produced by thermal cracking of EDC and this endothermic reaction was performed with respect to 108 reversible elementary reactions with 47 molecular and radical species. Pyrolysis reaction kinetics was derived from Choi *et al*, 2001.



Table A2 Elementary Reactions for EDC Pyrolysis (Forward Reactions Only)

Reaction	A	b	E
<b>Chain Initiation Reactions</b>			
$\text{CH}_2\text{ClCH}_2\text{Cl} = \text{CH}_2\text{ClCH}_2 + \text{Cl}$	1.01E28	-4.6	86509
$\text{C}_2\text{H}_3\text{Cl} = \text{C}_2\text{H}_3 + \text{Cl}$	1.71E38	-7.1	96370
$\text{CH}_2\text{Cl}_2 = \text{CH}_2\text{Cl} + \text{Cl}$	1.02E16	0	76800
$\text{CHCl}_3 = \text{CHCl}_2 + \text{Cl}$	0.6E16	0	71000
$\text{CCl}_4 = \text{CCl}_3 + \text{Cl}$	1E16	0	70000
$\text{CH}_3\text{Cl} = \text{CH}_3 + \text{Cl}$	1.26E37	-6.9	90540
$\text{C}_4\text{H}_6\text{Cl}_2 = \text{C}_4\text{H}_6\text{Cl} + \text{Cl}$	1E16	0	66600
$\text{C}_4\text{H}_5\text{ClS} = \text{C}_4\text{H}_5\text{S} + \text{Cl}$	1E16	0	85900
$\text{C}_4\text{H}_5\text{ClU} = \text{C}_4\text{H}_5\text{U} + \text{Cl}$	1E16	0	94900
$\text{C}_2\text{H}_5\text{Cl} = \text{C}_2\text{H}_5 + \text{Cl}$	1E16	0	86200
$\text{CH}_2\text{ClCHCl}_2 = \text{CH}_2\text{ClCHCl} + \text{Cl}$	1E13	0	77000
<b>H Abstraction Reactions</b>			
$\text{CH}_2\text{ClCH}_2\text{Cl} + \text{Cl} = \text{CH}_2\text{ClCHCl} + \text{HCl}$	1E13	0	3100
$\text{CH}_2\text{ClCH}_2\text{Cl} + \text{CH}_2\text{Cl} = \text{CH}_2\text{ClCHCl} + \text{CH}_3\text{Cl}$	1.16E11	0	9000
$\text{CH}_4 + \text{CH}_2\text{ClCHCl} = \text{CH}_2\text{ClCH}_2\text{Cl} + \text{CH}_3$	1E5	2	25933
$\text{C}_2\text{H}_3\text{Cl} + \text{CH}_2\text{Cl} = \text{CH}_2\text{CCl} + \text{CH}_3\text{Cl}$	1.79E1	3.6	9620
$\text{C}_2\text{H}_3\text{Cl} + \text{CH}_2\text{Cl} = \text{CHClCH} + \text{CH}_3\text{Cl}$	1.79E1	3.6	14480
$\text{C}_2\text{H}_3\text{Cl} + \text{Cl} = \text{CH}_2\text{CCl} + \text{HCl}$	1.2E14	0	13300
$\text{C}_2\text{H}_3\text{Cl} + \text{Cl} = \text{CHClCH} + \text{HCl}$	1.2E14	0	13300
$\text{CH}_2\text{ClCH}_2 + \text{CH}_3\text{Cl} = \text{C}_2\text{H}_5\text{Cl} + \text{CH}_2\text{Cl}$	1E6	2	11408
$\text{C}_2\text{H}_5\text{Cl} + \text{Cl} = \text{CH}_2\text{ClCH}_2 + \text{HCl}$	2.5E7	2	680
$\text{CH}_3\text{Cl} + \text{Cl} = \text{CH}_2\text{Cl} + \text{HCl}$	9.3E6	2.4	3300
$\text{CH}_3\text{Cl} + \text{CH}_3 = \text{CH}_2\text{Cl} + \text{CH}_4$	1.26E11	0	11600
$\text{CH}_4 + \text{Cl} = \text{CH}_3 + \text{HCl}$	2.08E8	1.8	2650
$\text{CH}_3\text{Cl} + \text{CHCl}_2\text{CHCl} = \text{CH}_2\text{ClCHCl}_2 + \text{CH}_2\text{Cl}$	1E6	2	14158
$\text{C}_2\text{H}_4 + \text{CH}_2\text{Cl} = \text{C}_2\text{H}_3 + \text{CH}_3\text{Cl}$	2E12	0	12000
$\text{C}_2\text{H}_3\text{Cl} + \text{CH}_3 = \text{CH}_2\text{CCl} + \text{CH}_4$	1.08E1	3.9	10490
$\text{C}_2\text{H}_3\text{Cl} + \text{CH}_3 = \text{CHClCH} + \text{CH}_4$	1.08E1	3.9	12490
$\text{C}_2\text{H}_3\text{Cl} + \text{CHCl}_2 = \text{CH}_2\text{Cl}_2 + \text{CHClCH}$	1E6	2	20158
$\text{C}_2\text{H}_3\text{Cl} + \text{CHCl}_2 = \text{CH}_2\text{Cl}_2 + \text{CH}_2\text{CCl}$	1E6	2	17608
$\text{C}_4\text{H}_4\text{Cl} + \text{HCl} = \text{C}_4\text{H}_5\text{ClS} + \text{Cl}$	1E6	2	18283

Reaction	A	b	E
$C_4H_5U + CH_3Cl = C_4H_6 + CH_2Cl$	1E5	2	21733
$C_4H_5Cl_2U + HCl = C_4H_6Cl_2 + Cl$	1E6	2	29833
$C_4H_5U + HCl = C_4H_6 + Cl$	1E6	2	23233
$C_4H_5S + CH_3Cl = C_4H_6 + Cl$	1E6	2	35158
$C_2H_4 + Cl = C_2H_3 + HCl$	1E14	0	7000
$C_2H_3Cl + CH_3 = CH_2ClCH_2 + CH_4$	4.4E2	3.2	10340
$C_2H_5Cl + CH_3 = CH_3CHCl + CH_4$	4.4E2	3.2	9340
$C_2H_3Cl + CHCl_2CHCl = CHClCH + CH_2ClCHCl_2$	1E6	2	22408
$C_2H_3Cl + CHCl_2CHCl = CH_2CCl + CH_2ClCHCl_2$	1E6	2	19858
$C_2H_3Cl + CHClCCl = CHClCH + CHClCHCl$	1E6	2	13708
$C_2H_3Cl + CHClCCl = CH_2CCl + CHClCHCl$	1E6	2	11358
$C_2H_3Cl + CH_2ClCH_2 = CHClCH + C_2H_5Cl$	1E6	2	19558
$C_2H_3Cl + CH_2ClCH_2 = CH_2CCl + C_2H_5Cl$	1E6	2	17008
$C_2H_3Cl + CH_3CHCl = CHClCH + C_2H_5Cl$	1E6	2	24616
$C_2H_3Cl + CH_3CHCl = CH_2CCl + C_2H_5Cl$	1E6	2	20608
$CH_2ClCHCl + C_2H_4 = CH_2ClCH_2Cl + C_2H_3$	1E6	2	19258
$CH_2ClCHCl + C_2H_6 = CH_2ClCH_2Cl + C_2H_5$	1E6	2	13408
$CH_2ClCHCl + C_2H_3Cl = CH_2ClCH_2Cl + CHClCH$	1E5	2	22408
$CH_2ClCHCl + C_2H_3Cl = CH_2ClCH_2Cl + CH_2CCl$	1E6	2	19858
$Cl + C_2H_6 = HCl + C_2H_5$	1E14	0	1000
$H + HCl = H_2 + Cl$	5.01E12	0	3200
$Cl + C_2H_2 = HCl + C_2H$	1.6E14	0	16900
$Cl + C_4H_4 = HCl + C_4H_3$	1E14	0	1000
<b>Cl Abstraction Reactions</b>			
$CH_2ClCH_2Cl + Cl = CH_2ClCH_2 + Cl_2$	1E7	2	28108
$CH_2ClCH_2Cl + CH_2Cl = CH_2ClCH_2 + CH_2Cl_2$	1E6	2	11283
$CH_2ClCH_2Cl + CH_3 = CH_2ClCH_2 + CH_3Cl$	4E5	2	16908
$CCl_4 + CH_3 = CCl_3 + CH_3Cl$	1.26E12	0	9900
$CCl_4 + Cl = CCl_3 + Cl_2$	1E14	0	20000
$C_2H_3Cl + CCl_3 = C_2H_3 + CCl_4$	1E6	2	27808
$C_4H_6Cl_2 + Cl = C_4H_6Cl + Cl_2$	1E7	2	17908
$C_4H_6ClS + Cl = C_4H_5S + Cl_2$	1E7	2	27900
$C_4H_6ClU + Cl = C_4H_5U + Cl_2$	1E7	2	36900
$C_4H_5U + HCl = C_4H_5ClU + H$	1E6	2	28858
$C_4H_5S + HCl = C_4H_5ClS + H$	1E6	2	41533

Reaction	A	b	E
$C_2H_3Cl + CHClCH = C_2H_3 + C_2HCl_3$	1E6	2	14233
$C_2H_3Cl + CH_2CCl = C_2H_3 + CCl_2CH_2$	1E6	2	13783
$C_2H_3Cl + CH_2ClCH_2 = C_2H_3 + C H_2ClCH_2Cl$	1E6	2	17758
$CH_3 + C_2H_3Cl = CH_3Cl + C_2H_3$	3E11	0	17983
$Cl_2 + C_2H_3 = C_2H_3Cl + Cl$	5.24E12	0	-480
$CH_2ClCHCl + CH_3Cl = CH_2ClCHCl_2 + CH_3$	1E11	0	17950
$CH_3CHCl_2 + CH_2ClCHCl = CH_3CHCl + CH_2ClCHCl_2$	1E6	2	16783
$C_2H_3Cl + CH_3CHCl = C_2H_3 + CH_3CHCl_2$	1E6	2	21508
$CH_2ClCHCl + C_2H_3Cl = CH_2ClCHCl_2 + C_2H_3$	1E12	0	18550
$CH_2ClCHCl + Cl_2 = CH_2ClCHCl_2 + Cl$	1E12	0	6175
<b>Radical Addition Reactions</b>			
$C_2H_2 + C_2H_3 = C_4H_5U$	7.94E8	0	6900
$C_2H_2 + C_2H_3 = C_4H_5S$	7.94E8	0	6900
$C_2H_3Cl + C_2H_3 = C_4H_6Cl$	2.28E27	-4.6	11778
$C_2H_3Cl + C_2H_3 = C_4H_6 + Cl$	2.13E8	1.7	9157
$C_2H_3Cl + CH_2CCl = C_4H_5ClS + Cl$	7.94E13	0	12844
$CH_3 + C_2H_4 = C_3H_7$	1E12	0	2000
$CH_3 + C_3H_6 = (CH_3)_2CHCH_2$	6.31E11	0	8800
$C_2H_3 + C_2H_4 = C_4H_7$	2E11	0	2000
$C_2H_3 + C_4H_6 = C_6H_9$	3.2E11	0	3000
$C_4H_5 + C_2H_2 = C_6H_7$	3.98E12	0	6900
$C_2H_3 + c-C_6H_6 = C_6H_6C_2H_3$	1.58E11	0	3000
<b>Radical decomposition Reactions</b>			
$CH_2ClCHCl = C_2H_3Cl + Cl$	1.58E13	0	20600
$CHClCCl = C_2HCl + Cl$	3.82E28	-5	37441
$CHClCH = C_2H_2 + Cl$	1.5E13	0	23000
$C_4H_5Cl_2U = C_4H_5ClU + Cl$	3E13	0	37000
$C_4H_6Cl = C_4H_6 + Cl$	3E13	0	41600
$C_2H_5 = C_2H_4 + H$	2E13	0	39100
$C_3H_7 = C_3H_6 + H$	6.31E13	0	38000
$(CH_3)_2CHCH_2 = (CH_3)_2CCH_2 + H$	1E14	0	36300
$C_4H_7 = C_4H_6 + H$	3.2E13	0	34800
$C_4H_5 = C_4H_4 + H$	1E14	0	41400

Reaction	A	b	E
$C_6H_9 = C_6H_8 + H$	3.2E13	0	42200
$c-C_6H_9 = c-C_6H_8 + H$	6.31E7	0	34300
$C_6H_6C_2H_3 = C_6H_5C_2H_3 + H$	5.01E13	0	26000
$C_4H_3 = C_4H_2 + H$	1E14	0	40800
$C_2H_3 = C_2H_2 + H$	1E14	0	40400
$c-C_6H_7 = c-C_6H_6 + H$	1E14	0	15000
<b>Pure Radical Reactions</b>			
$CH_2CCl + C_2H_3 = C_4H_5S + Cl$	3.46E11	0	10443
$C_2H_3 + CH_2ClCHCl = C_4H_6Cl + Cl$	1.41E14	0	10416
$C_6H_9 = c-C_6H_9$	2E11	0	8000
$C_6H_7 = c-C_6H_7$	3.16E11	0	8000
<b>Pure Molecular Reactions</b>			
$CH_2ClCH_2Cl = C_2H_3Cl + HCl$	1.43E12	-0.7	58920
$C_2H_3Cl = C_2H_2 + HCl$	2.75E17	-1.3	69312
$C_4H_6Cl_2 = C_4H_5ClS + HCl$	3.98E10	0	49000
$C_4H_6Cl_2 = C_4H_5ClU + HCl$	3.98E10	0	51000
$C_2H_5Cl = C_2H_4 + HCl$	3.2E13	0	57600
$C_6H_8 = C_6H_6 + H_2$	3.2E13	0	40000
$c-C_6H_8 = c-C_6H_6 + H_2$	2.51E12	0	43800
<b>Chain Termination Reactions</b>			
$CH_2Cl + CH_2Cl = CH_2ClCH_2Cl$	3E38	-8	9431
$CH_2ClCHCl + Cl = CHClCHCl + HCl$	1E8	2	0
$CHClCCl + Cl = C_2Cl_2 + HCl$	1E8	2	3080
$CH_2Cl + CH_2Cl = C_2H_3Cl + HCl$	1.1E24	-3.2	8200
$CH_2ClCH_2 + Cl = C_2H_3Cl + HCl$	1.1E30	-4.7	17464
$C_2H_3 + Cl = C_2H_2 + HCl$	4.7E25	-3.2	11790
$C_2H_3 + CH_2Cl = C_2H_2 + CH_3Cl$	1E13	0	0
$C_2H_3 + CH_2ClCHCl = C_4H_5ClS + HCl$	1.98E13	0	7127
$C_2H_3 + CH_2ClCHCl = C_4H_5ClU + HCl$	1.98E13	0	7127
$CH_2CCl + C_2H_3 = C_4H_5ClS$	1.29E12	0.4	1565
$C_4H_5Cl_2S + Cl = C_4H_4Cl_2 + HCl$	1E7	2	0
$C_4H_5Cl_2S + Cl = C_4H_4ClS + Cl_2$	1E7	2	0
$C_4H_5Cl_2U + Cl = C_4H_4Cl_2 + HCl$	1E7	2	0
$C_4H_5Cl_2U + Cl = C_4H_4ClU + Cl_2$	1E7	2	0



**TableA3** Pyrolysis effluent fractions

Chemicals	Fraction of effluent components
VCM	3.95E-01
HCl	3.97E-01
EDC	2.07E-01
chloroprene	1.72E-14
acetylene	3.06E-04
ethylene	1.91E-05
TCE	1.24E-11
CH <sub>3</sub> Cl	1.39E-06
1,1-dichloroethylene	1.44E-06
1,2-dichloroethylene	7.14E-07
Chloroethane	2.98E-07
CH <sub>2</sub> Cl <sub>2</sub>	4.60E-08
butadiene	4.55E-08
Cl <sub>2</sub>	2.48E-09
trichloroethylene	1.88E-09

## Appendix B Sizing and cost estimation of equipment.

### Thermal Incineration

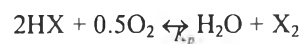
#### 1. Thermal incinerator system design

The reactions of combustion (complete combustion)

Ethylene burns as follows:  $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$

Ethylene Dichloride may burns as follows:  $C_2H_4Cl_2 + 3O_2 \rightarrow 2CO_2 + 2H_2O + Cl_2$

In the incineration environment, the halogen acids (HX) and the free elements ( $X_2$ ) are in dynamic equilibrium with water vapor and oxygen (the Deacon reaction) in Niessen, 2002 according to



$$K_p = \frac{P_{H_2O} P_{X_2}}{P_{HX}^2 P_{O_2}^{1/2}} \text{ atm}^{-1/2}$$

The temperature dependence of  $K_p$  (for partial pressure in atm and temperature (T) in K is given by

$$\text{Chlorine In } K_p = -8.244 + 1.512 \cdot 10^{-4} T + 7087/T$$

However, the incinerator system have large amount of oxygen excess, so occurring HCl can neglect.

$$\tau = \left( \frac{V}{Q} \right)$$

where

$\tau$  = residence time

$V$  = internal volume of the incinerator chamber

$Q$  = flow rate of gases out of the incinerator

#### The total flue gas flow

$$Q = Q_w + Q_f$$

where

$Q$  = Total flue gas flow rate

$Q_w$  = Waste gas flow rate at inlet to incinerator

$Q_f$  = Flow rate of auxiliary fuel

#### The flow rate of auxiliary fuel

$$Q_f = Q_w X/Y$$

where

$$X = 1.1 C_{po} (T_c - T_r) - C_{pi} (T_r - T_r) - h_w$$

$$Y = h_f - 1.1 C_{po} (T_c - T_r)$$

$C_{po}$  = mean heat capacity of exhaust stream from the incinerator

$T_c$  = combustion temperature

- $T_r$  = reference temperature  
 $C_{pi}$  = mean heat capacity of inlet streams to the incinerator  
 $T_i$  = inlet gas stream temperature, after preheating.  
 $T_i$  may be calculated from the equation  $T_i = T_w + \text{Eff} (T_c - T_w)$   
 $T_w$  = temperature of waste gas stream before preheating  
 $\text{Eff}$  = anticipated fractional thermal efficiency of the incinerator  
 $h_w$  = heat content of waste gas stream  
 $h_f$  = heat content of fuel

These equations are considered valid for gas streams with an oxygen content above 16% that contain VOCs at a concentration less than 25% of the LEL. They assume a 10% loss of energy from the incinerator.

## 2. Economic Estimates

The capital cost of a package recuperative thermal incineration system (Hunter *et al*, 2000)

$$CC = a (Q)^b$$

where

- $CC$  = purchased price, in 1988 (dollars)  
 $Q$  = flow rate of gases after combustion ( $\text{ft}^3/\text{min}$ )

At 70% heat recovery,  $a = 5.690$  and  $b = 0.408$

## Absorption System

### 1. Absorption system design (Hunter *et al*, 2000)

#### Design Procedures for Packed Columns Separating Dilute Solutes

$$\frac{L_M}{G_M} \left( \frac{\rho_G}{\rho_L} \right)^{0.5}$$

where

- $L_M$  = liquid flow rate, mass/h units  
 $G_M$  = gaseous flow rate, mass/h units  
 $\rho_G$  = gas density, 0.073  $\text{lb}/\text{ft}^3$  for air at 303 K  
 $\rho_L$  = liquid density, 62.4  $\text{lb}/\text{ft}^3$  for water at 303 K

$$G'_{flood} = \frac{[\varepsilon \rho_G \rho_L g_c]^{0.5}}{[F \phi \mu_L^{0.2}]^{0.5}}$$

where

$G'_{flood}$  = the mass flow rate of gas per unit of column cross-sectional area that will just cause the column to flood,  $\text{lb s}^{-1}\text{ft}^{-2}$

- $\varepsilon$  = the y-axis value from Fig. 5.8 in Hunter *et al*, 2000  
 $g_c$  = the gravitational constant, 32.2  $\text{ft}/\text{s}^2$



$\phi$  = ratio of liquid specific gravity to that of water

$\mu_L$  = liquid viscosity, cP, 0.8 cP for water

Assume 75% of flooding,

$$G_{oper}^+ = 0.75G_{flood}^+$$

where

$G_{oper}^+$  = mass flow of gas stream per unit area of column under normal operation,  
(lb s<sup>-1</sup>ft<sup>-2</sup>)

The required column cross-sectional area,

$$A = G / G_{oper}^+$$

where

A = the cross-sectional area, ft<sup>2</sup>

Calculating the column diameter from

$$D = \left( \frac{4A_c}{\pi} \right)^{1/2}$$

where

D = the diameter of the column

$$N_{OG} = \frac{\ln \left\{ \left[ \frac{(A-1)}{A} \right] \left[ \frac{(Y_i - KX_i)}{(Y_0 - KX_i)} \right] + \frac{1}{A} \right\}}{(A-1)/A}$$

where

$Y_0$  = pollutant concentration in gas stream leaving absorber, kg-mol pollutant/kg-mol  
pollutant-free gas (lb-mol/lb-mol)

$Y_i$  = pollutant concentration in gas stream entering absorber, kg-mol pollutant/kg-mol  
pollutant-free gas (lb-mol/lb-mol)

$X_i$  = concentration of pollutant in liquid stream entering the absorber kg-mol  
pollutant/kg-mol pollutant-free solvent (lb-mol/lb-mol)

A = L/KV

L = liquid flow rate

V = gas flow rate

The height of a theoretical transfer unit ( $H_{OG}$ ) should be obtained from vendor information for the specific application, but it usually ranges between 0.3 and 1.2 m (1 and 4 ft). A rough estimation of 0.6 m (2ft) can be used if necessary.

$$D = \left( \frac{4A_c}{\pi} \right)^{1/2}$$

The total packing height is calculated from

$$H_{pack} = N_{OG} \cdot H_{OG}$$

## 2. Economic Estimates

The total column surface area is first calculated:

$$S = \pi D(1.4H_{pack} + 1.52D + 2.81)$$

where

$S$  = surface area of column, ft<sup>2</sup>

The cost of adsorption system (in third-quarter 1991 \$) can be estimated by:

$$\text{Cost (\$)} = S(\text{ft}^2) * 115(\$/\text{ft}^2)$$

## Appendix C Forecasted value and reference data.

### Forecasted value

**Table C1** Forecasted demand of vinyl chloride monomer (,000T/Y) in Thailand

year	demand	capacity	demand-capacity
1996	402	280	122
1997	489	300	189
1998	478	600	-122
1999	538	600	-62
2000	605	615	-10
2001	645	627	18
2002	670	627	43
2003			96
2004			137
2005			178
2006			219
2007			260
2008			301
2009			342
2010			383
2011			424
2012			465
2013			506
2014			547
2015			588
2016			629
2017			670
2018			711
2019			752
2020			793
2021			834
2022			875
2023			916
2024			957
2025			958
2026			1039

Demands of VCM (Petroleum Institute of Thailand) are plotted between demands of VCM (,000T/Y) vs. year from 1998-2002 to determine forecast demand of VCM.

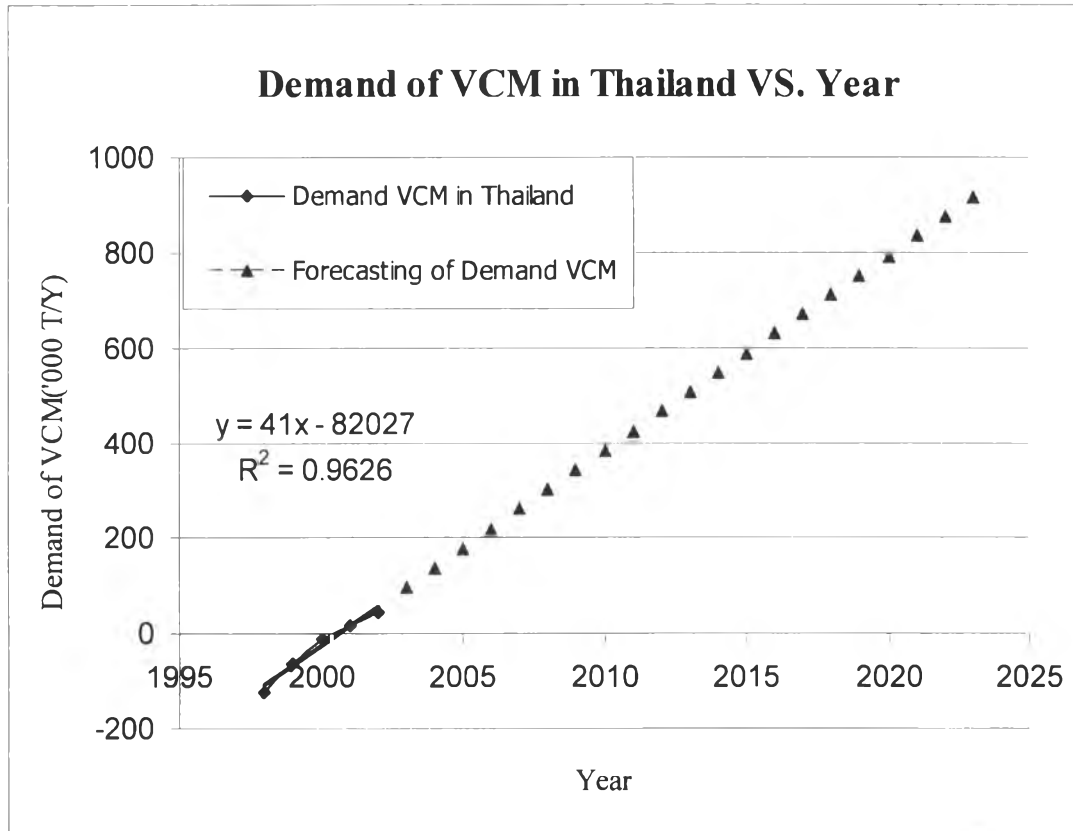
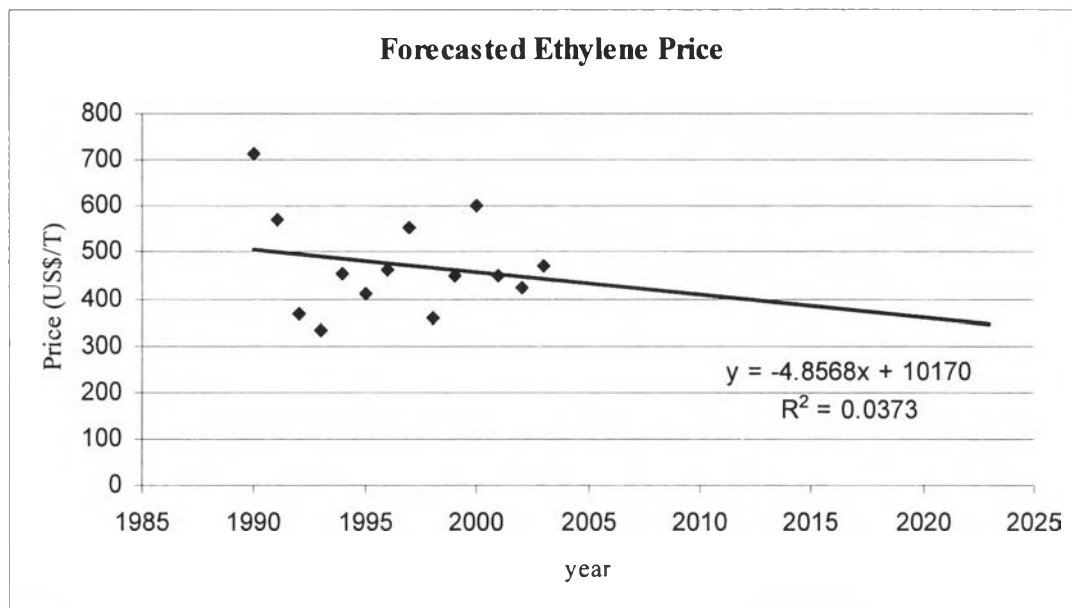


Figure C1 Demand of VCM in Thailand.

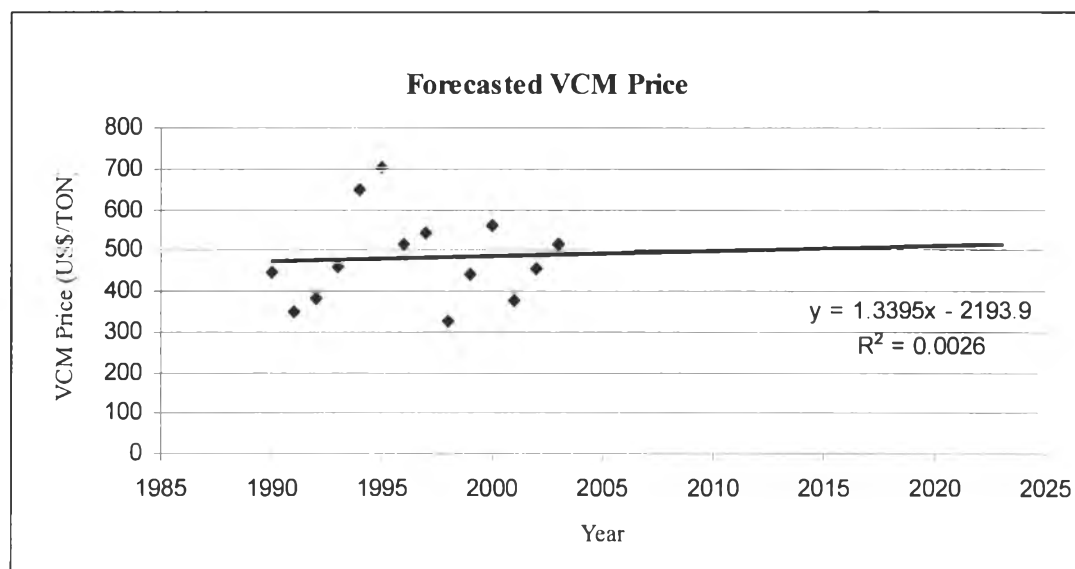
**Table C2** Forecasted Prices and random values of vinyl chloride monomer, ethylene (Thai Olefins Co.,Ltd.)

Unit: US\$/Ton

Year	Ethylene price	Vinyl chloride monomer price
1990	715.08	445.91
1991	570.08	347.90
1992	366.33	383.08
1993	331.25	459.73
1994	455.50	648.08
1995	410.67	705.00
1996	464.42	514.79
1997	552.75	543.75
1998	357.75	326.67
1999	451.08	440.83
2000	602.50	562.29
2001	450.42	378.54
2002	422.29	455.00
2003	472.99	514.88
2004	436.97	490.46
2005	432.12	491.80
2006	427.26	493.14
2007	422.40	494.48
2008	417.55	495.82
2009	412.69	497.16
2010	407.83	498.50
2011	402.98	499.83
2012	398.12	501.17
2013	393.26	502.51
2014	388.40	503.85
2015	383.55	505.19
2016	378.69	506.53
2017	373.83	507.87
2018	368.98	509.21
2019	364.12	510.55
2020	359.26	511.89
2021	354.41	513.23
2022	349.55	514.57
2023	344.69	515.91
2024	339.84	517.25
2025	334.98	518.59
2026	330.12	519.93
<b>Standard Error</b>	<b>107.38</b>	<b>114.06</b>



**Figure C2** Forecasted prices of ethylene.



**Figure C3** Forecasted prices of VCM.

**Reference data****Table C3** Reference data

Data	Reference
Chlorine price = 210.4 \$/ ton Oxygen price = 40 \$/ton HCl price = 273 \$/ton 1 US\$ = 39.83 Bath Land rent in Map Ta Phut = 30,360 Bath/Rai/year Labor Cost = 17,684 Bath/month	Peters <i>et al</i> , 2003 Peters <i>et al</i> , 2003 Peters <i>et al</i> , 2003 October 11, 2003. Map Ta Phut Office.  Fiscal year 2000-2001 Data of Average Wages Type in Rayong. Labour studies and planning division in department of labour protection and welfare.
Coal properties <ul style="list-style-type: none"> <li>• Heating value = 8250 kcal/kg</li> <li>• Composition of               <ul style="list-style-type: none"> <li>C =93.9%</li> <li>H<sub>2</sub> = 2.1%</li> <li>O<sub>2</sub> = 2.3%</li> <li>S = 0.9%</li> <li>N<sub>2</sub> = 0.3%</li> </ul> </li> </ul>	Coal from Schuylkill, USA in Table 2 and 3 in App. B in Niessen et al, 2002

## Appendix D The method of calculations of financial and environmental risks.

The method of calculations of financial and environmental risk for VCM plant at capacity of 300,000 ton/year and 50% HCl recycle with heat integration and the treatment system.

### Equipment Cost

The major equipment of the VCM plant consists of three reactors, heat exchangers, four distillation towers, eight flash tanks, carbon adsorption system, a regeneration unit, an incinerator, and absorption column. The equipment price values is found in Peters *et al*, 2003, and Hunter *et al*, 2000 and using Chemical Engineering plant cost index<sup>1</sup> to update the price.

#### Reactors

Stainless steel was selected material used for all of the reactors. Oxychlorination reactor (RX2) was treated as plug flow tubular reactors (PFTR) considered shell and tube heat exchangers. The cracking reactor (PYRO) was treated a furnace. The duty of the reactor is used to determine the cost.

**Table D1** Reactor Cost

Name	Types	Cost (\$) (Jan2002)	Cost Reference	Cost (\$) (Aug2004)
RX1	CSTR	2,235,000	Fig.12-52, Peters <i>et al</i> , 2003	2,303,699
RX2	PFTR	60,000	Fig.14-17, Peters <i>et al</i> , 2003	61,844
PYRO	Cracking	440,000	Fig.14-37, Peters <i>et al</i> , 2003	453,525

#### Distillation Column

Tray type selected is sieve tray with tray spacing of 24 in because this type is suitable for high pressure and high liquid flow rate operating conditions when the column diameter is large. Sieve trays are the choice in many distillation separations since its tray fundamentals are well established, entailing low risk. In addition, the trays are low in cost relative to many other tray types while handling wide variations in flow rates. Using the correlation of column diameter to cost per tray from Figure 15-13 in Peters *et al*, 2003, the cost of the distillation columns was estimated.

<sup>1</sup> Chemical Engineering, November 2003, p.124.



**Table D2** Distillation Column Cost

Parameters	Distillation			
	Col 1	Col 2	Col 3	Col 4
Number of Tray	15	28	40	18
Diameter (m)	0.126	2.91	1.08	1.20
Height (m)	13.04	20.97	28.29	14.87
Purchased & Installed cost (\$/tray)	300	1,300	500	500
Quantity factors	1.25	1	0.97	1.1
Purchased & Installed cost (\$) (Jan2002)	5,625	36,400	19,400	14850
Purchased & Installed cost (\$) (Aug2003)	5798	37,519	19,996	8,998

#### Heat Integration Design and Heat Exchanger Cost

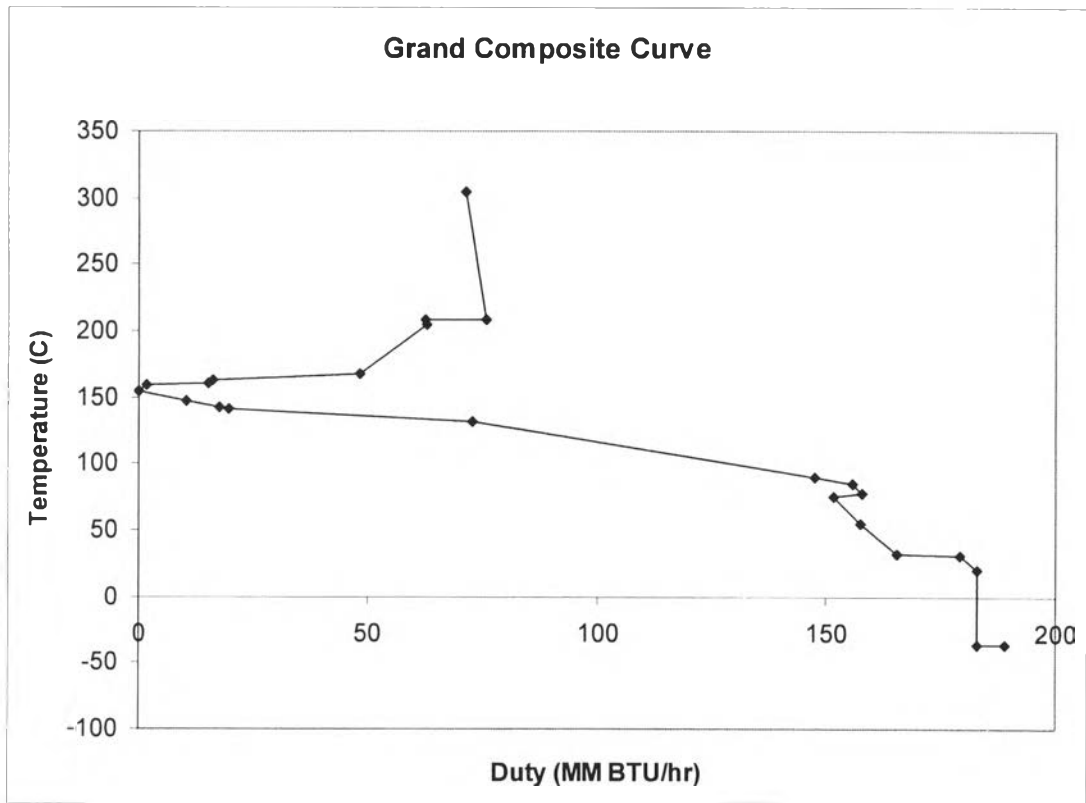
Heat Integration Design: The VCM plant process design including a heat-integrated network assumes a minimum approach temperature ( $\Delta T_m$ ) of 10 °C for efficient heat exchange. Based on the stream data and the temperature targets are required for the process, and a table cascade was constructed to find the minimum utilities by using the pinch method. These utilities include all heat exchangers, all of the column reboilers and the column condensers. The heat capacity data for the individual streams is given in Table D2 to set up the grand composite curve for the system (see Figure D1).

**Table D3** Data for the heat exchanger network in the vinyl chloride case study

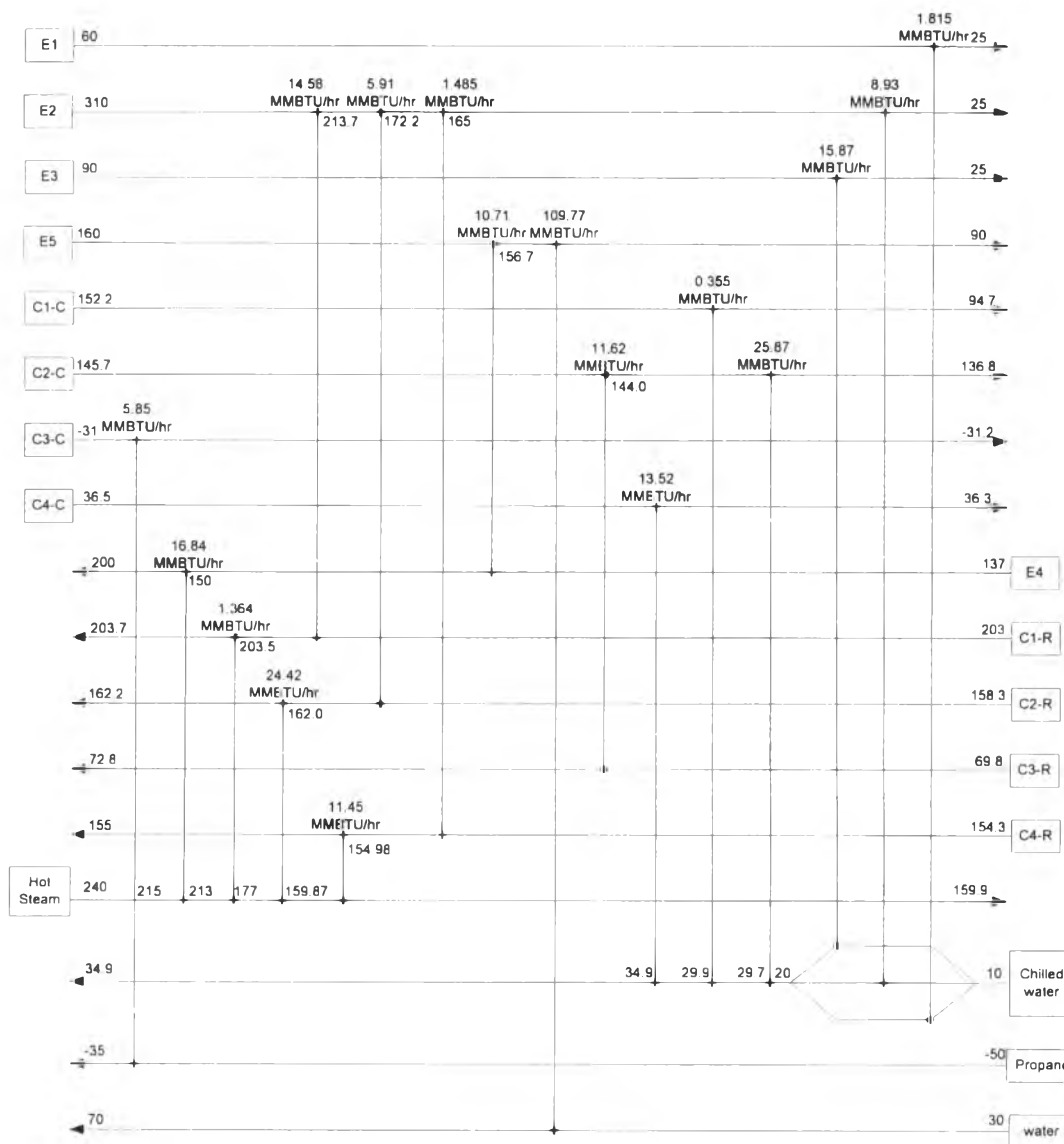
Stream	Description	T <sub>in</sub> (°C)	T <sub>out</sub> (°C)	F (MM BTU/hr/°C)
E1	-	60	25	0.052
E2	-	310	25	0.046
E3	-	90	25	0.244
E5	-	160	90	1.721
C1-C	Condenser of the COL1	152.2	94.7	0.006
C2-C	Condenser of the COL2	145.7	136.8	4.213
C3-C	Condenser of the COL3	-31	-31.2	29.27
C4-C	Condenser of the COL4	36.5	36.3	67.61
E4	-	137	200	0.4374
C1-R	Reboiler of the COL1	203	203.7	18.876
C2-R	Reboiler of the COL2	158.3	162.2	7.7773
C3-R	Reboiler of the COL3	69.8	72.8	2.3206
C4-R	Reboiler of the COL4	154.3	155	18.477

From the grand composite curve (Figure D1), the minimum hot utility is 71.49 MMBTU/hr, and minimum cold utility is 188.9 MMBTU/hr. The pinch temperature is equal to 160°C. The overall energy requirements of the plant of all equipment reduced from 149.11 to 104.61 MMBTU/hr for the hot utility, and reduced from 208.42 to 163.92 MMBTU/hr for the cold utility which the heat exchanger network for the process streams present in Figure D2.

The Figure D2 shows the optimal heat exchanger network. The intermediate utilities (chilled water, steam and water) were not considered as process streams. Nine hot streams (E1-E3, E5, C1-C, C2-C, C3-C, C4-C, hot steam) and eight cold streams (E4, C1-R, C2-R, C3-R, C4-R, chilled water, propane and water) were included in the network.



**Figure D1** Grand Composite Curve.



**Figure D2** Heat exchange network for the process streams.

Heat Exchanger Cost: The overall heat-transfer coefficients ( $U_d$ ) was assume from the hot and cold fluid used for each heat exchanger (Peters *et al*, 2003). To estimate the costs of heat exchangers, the correlation of surface area to purchase cost from Figure 14-17 in Peters *et al*, 2003 was used. From Figure D2, The heat exchanger cost is equal to \$419,576.

Flash Tank Cost

Using the graph of capacity obtained from the liquid flow rate leaving the vessel to purchased cost from Figure 12-52 in Peters *et al*, 2003, the costs of the flash tanks was estimated.

**Table D3** Flash Tank Cost

Name	Leaving of Liquid Flow Rate (ft <sup>3</sup> /hr)	Residence time (hr)	Volume (ft <sup>3</sup> )	Cost (\$) (Jan2002)	Cost (\$) (Aug2003)
DC-FLASH	1104.42	0.08	92.04	2.61	16,000
OXY-FLASH	440.30	0.08	36.69	1.04	10,000
FLS3	1486.08	0.08	123.84	3.51	19,000
FLS4	2209.40	0.08	184.12	5.21	24,000
FLS5	12360.17	0.08	1,030.01	29.17	60,000
FLS6	11873.19	0.08	989.43	28.02	60,000
FLS7	2257.58	0.08	188.13	5.33	24,000
DC-CAUS	9.65	0.08	0.80	0.02	2,900

#### Incineration Unit

Incineration system is treatment unit to eliminate or reduce vapor and liquid byproduct before release to the atmosphere. The cost of incineration unit can be estimated by using a package recuperative thermal incineration system method described in Hunter *et al*, 2000 and shown in Appendix B. The cost of incineration unit was obtained from the flow rate of gases after combustion.

**Table D4** Incineration unit cost

Incineration Unit	
Flow rate of gases after combustion(ft <sup>3</sup> /min)	288,337.7
Cost of Incineration system (\$, 1988)	961,063
Cost of Incineration system (\$, Aug2003)	1,127,000

#### Carbon Adsorption Column and Regeneration Unit

Wastewater was treated by carbon adsorption system. Using the correlation of the capacity of sewage to purchased cost of carbon adsorption from Figure B-8 in Peters *et al*, 2003, the cost of the incineration unit were estimated.

**Table D5** Carbon adsorption column and regeneration cost

Carbon Adsorption System	
Capacity of waste water (m <sup>3</sup> /s)	0.01289
Cost (\$, Jan2002)	720,236
Cost (\$, Aug2003)	742,374

#### Absorption System

Absorption system is used to remove contaminants in the plant exhaust before it is release into the atmosphere. The cost of absorption unit can be estimated by using a method described in Hunter *et al*, 2000, and is considered to be accurate to within 30% shown in Appendix B.

**Table D6** Absorption system cost

Absorption System	
Diameter of the column (ft)	12.18
The total packing height (ft)	7.462
The total column surface area (ft <sup>2</sup> )	1216.74
Cost (\$, the third-quarter 1991)	139,925
Cost (\$, August 2003)	155,713

### Financial and Environmental Risk Curves

Mass and energy information obtained from the process simulator ProII provide financial and environmental risks by using the GAMS program to create scenarios. The keyword input file of ProII and GAMS program for VCM plant is shown in Appendix F.

The result from GAMS program is shown in Table D7 which is set the number of scenarios of 1000 scenarios. This data is manipulated to set up NPW histogram and its risk and EI histogram and its risks in Figure D3, and Figure D4, respectively.

Table D7 The result from GAMS program

Financial			Environmental			
NPW (\$)	Frequency	Cumulative %	IE (EIU/ton of VCM)	Frequency	Cumulative %	Risk %
-381,950,000	1	.10%	4.0076	1	.10%	99.90%
-354,489,871	0	.10%	4.12459677	0	.10%	99.90%
-327,029,742	0	.10%	4.24159355	2	.30%	99.70%
-299,569,613	4	.50%	4.35859032	3	.60%	99.40%
-272,109,484	2	.70%	4.4755871	6	1.20%	98.80%
-244,649,355	3	1.00%	4.59258387	5	1.70%	98.30%
-217,189,226	6	1.60%	4.70958065	16	3.30%	96.70%
-189,729,097	8	2.40%	4.82657742	24	5.70%	94.30%
-162,268,968	8	3.20%	4.94357419	31	8.80%	91.20%
-134,808,839	16	4.80%	5.06057097	37	12.50%	87.50%
-107,348,710	14	6.20%	5.17756774	61	18.60%	81.40%
-79,888,581	25	8.70%	5.29456452	49	23.50%	76.50%
-52,428,452	27	11.40%	5.41156129	69	30.40%	69.60%
-24,968,323	37	15.10%	5.52855806	92	39.60%	60.40%
2,491,806	53	20.40%	5.64555484	86	48.20%	51.80%
29,951,935	67	27.10%	5.76255161	60	54.20%	45.80%
57,412,065	63	33.40%	5.87954839	67	60.90%	39.10%
84,872,194	66	40.00%	5.99654516	63	67.20%	32.80%
112,332,323	96	49.60%	6.11354194	56	72.80%	27.20%
139,792,452	90	58.60%	6.23053871	49	77.70%	22.30%
167,252,581	75	66.10%	6.34753548	56	83.30%	16.70%
194,712,710	65	72.60%	6.46453226	30	86.30%	13.70%
222,172,839	70	79.60%	6.58152903	32	89.50%	10.50%
249,632,968	48	84.40%	6.69852581	30	92.50%	7.50%
277,093,097	45	88.90%	6.81552258	17	94.20%	5.80%
304,553,226	36	92.50%	6.93251935	14	95.60%	4.40%
332,013,355	21	94.60%	7.04951613	15	97.10%	2.90%
359,473,484	21	96.70%	7.1665129	10	98.10%	1.90%
386,933,613	11	97.80%	7.28350968	10	99.10%	.90%
414,393,742	13	99.10%	7.40050645	5	99.60%	.40%
441,853,871	4	99.50%	7.51750323	2	99.80%	.20%
More	5	100.00%	More	2	100.00%	.00%

E(NPW), \$ = 110,765,996  
S.D., \$ = 138,471,273

E(EI), EIU/ton of VCM = 5.75  
S.D. = 0.62

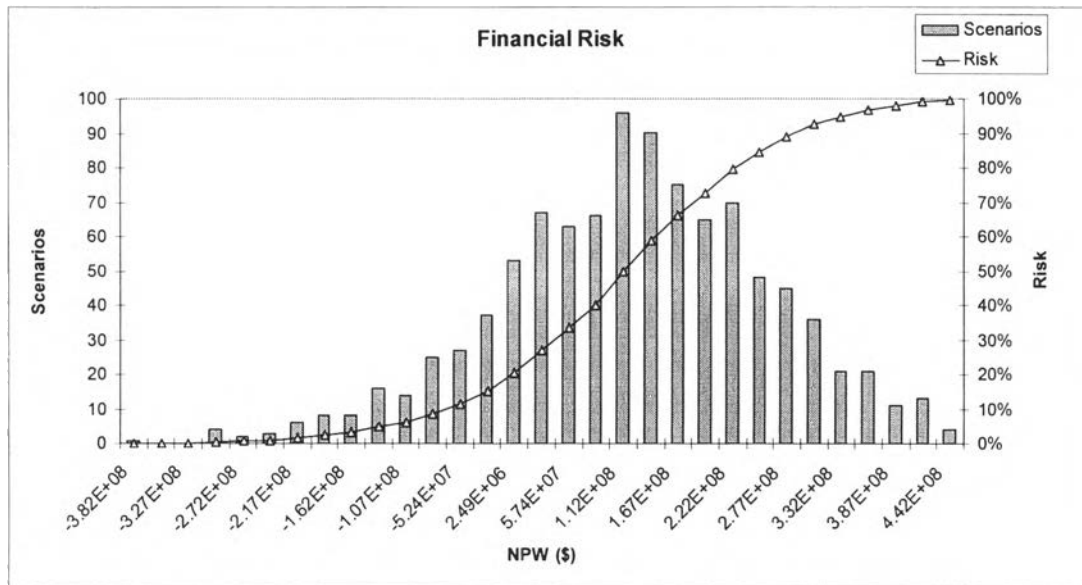


Figure D3 NPW histogram and financial risk.

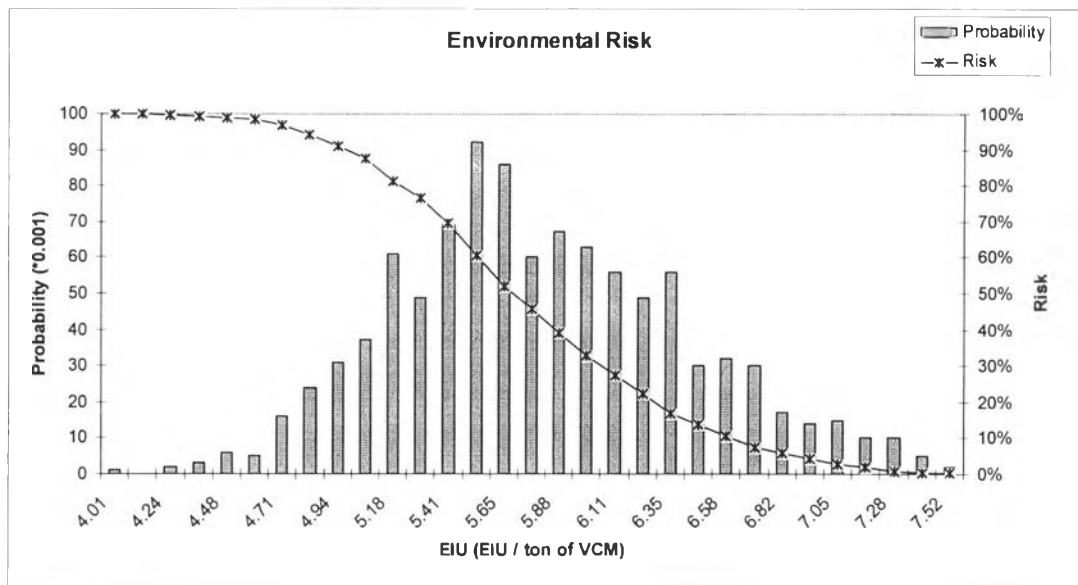


Figure D4 Environmental impact histogram and environmental risk.



## Appendix E Potential environmental impact.

A summary of their methodology for determining these parameters would be presented here.

### Global atmospheric impact categories

The GWP is determined by comparing the extent to which a unit mass of a chemical absorbs infrared radiation over its atmospheric lifetime to the extent that CO<sub>2</sub> absorbs infrared radiation over its respective lifetimes. The half-lives of each of these chemicals was factored into the calculation for determining the GWP. Since, chemicals have different atmospheric half-lives the length of time over which the comparison is made will change the GWP of a chemical. For the database, 100 years was chosen as the base time frame.

The ODP is determined by comparing the rate at which a unit mass of chemical reacts with ozone to form molecular oxygen to the rate at which a unit mass of CFC-11 (trichlorofluoromethane) reacts with ozone to form molecular oxygen.

For a chemical to have ODP it must exist in the atmosphere long enough to reach the stratosphere, it, also, must contain a chlorine or bromine atom.

The PCOP or smog formation potential is determined by comparing the rate at which a unit mass of chemical reacts with a hydroxyl radical (OH·) to the rate at which a unit mass of ethylene reacts with OH·.

The AP or acid rain potential is determined by comparing the rate of release of H<sup>+</sup> in the atmosphere as promoted by a chemical to the rate of release of H<sup>+</sup> in the atmosphere as promoted by SO<sub>2</sub>.

The values reported by Davis *et al* (1994) determine the chemical potential environmental impacts of these four categories.

### Local toxicological impact categories

Two categories were used to estimate the potential for human toxicity: ingestion and inhalation/dermal exposure. These two categories were used to estimate toxicity potential because they considered all of the primary routes of exposure of a chemical. As a general rule, HTPI were calculated for a chemical if it existed as a liquid or solid at a temperature of 0°C and atmospheric pressure, and an exposure potential, HTPE, was determined for that chemical if it existed as a gas at those conditions. Some chemicals, however, were assigned values for both categories if it was warranted.

As a first approximation, the lethal-dose that produced death in 50% of rats by oral ingestion (LD<sub>50</sub>) was used as an estimate for the HTPI. The value was chosen because of its prevalence in the literature and acceptance as a standard toxicity indicator. By inspection of this scale, it is quite apparent that a chemical with a higher LD<sub>50</sub> represents a chemical with lower toxicity. This scale is inverted from the manner in which the WAR algorithm is presented where a higher score represents a greater potential environmental impact.

This inversion assigns scores to chemicals in the database so that the more toxic chemicals have higher scores which follow with the concepts of the WAR algorithm. This inversion also maintains a proportional relationship between chemicals. For example, a chemical with an LD<sub>50</sub> of 200 mg/kg, producing a (Score)<sub>HTPI</sub> = 0.005, is considered to be twice as harmful as a chemical with an LD<sub>50</sub> of 400 mg/kg, producing a (Score)<sub>HTPI</sub> = 0.0025. The TTP was also estimated using this same rat-oral LD<sub>50</sub> data in exactly the same manner.

To estimate the HTPE, time-weighted averages (TWA) of the threshold limit values (TLV) were used. These values were obtained from OSHA, ACGIH, NIOSH and represent occupational safety exposure limits. This was considered to be an adequate measuring stick for comparison of chemicals that would pose a threat to human health through inhalation and dermal exposure routes. Recall, only a relative comparison within categories is needed for this methodology. Again, these values were inverted to maintain the proper relationships within the database. These estimations of human toxicity potential should be considered to be a first-order approximation only. However, for the time being the LD<sub>50</sub> values will be used to provide a relative toxicity comparison for both human and terrestrial entities. The ATP was estimated by using toxicological data for a single, representative species of fish. The data for this assay comes in the form of a LC<sub>50</sub>, a lethal concentration which causes death in 50% of the test specimens. The data used in this database specifically comes from 96 h, LC<sub>50</sub> experiments.

Tables E1 and E2 show the values of chemical k on some arbitrary scale for category l and the specific potential environmental impact of chemical k for impact category l, respectively, which is used as reference value to calculate environmental impact of designs.

**Table E1** The value of chemical k on some arbitrary scale for category l

Chemicals , k	$(Score)_{k,l}$						
	GWP	ODP	AP	PCOP	HTPI, TTP	HTPE	ATP
					1/LD <sub>50</sub>		
Ethylene				1.00E+00			7.14E-02
Chlorine						2.00E+00	2.94E+00
EDC				2.10E-02	1.49E-03	1.00E-01	7.35E-03
VCM				2.10E-02	2.00E-03	2.00E-01	6.99E-03
TCE	1.00E+02	1.20E-01		2.10E-02	1.77E-04	2.00E-02	2.27E-02
HCl			8.80E-01			2.00E-01	5.26E-02
SO <sub>2</sub>			1.00E+00			5.00E-01	
CO <sub>2</sub>	1.00E+00					2.00E-04	
$\langle (Score)_{k,l} \rangle$	5.05E+01	1.20E-01	9.40E-01	2.66E-01	1.22E-03	4.31E-01	5.17E-01

**Table E2** The specific potential environmental impact of chemical k for impact category I

Chemicals, k	$\Psi_{kl}^s$ (EIU/ton of VCM)						
Ethylene	0	0	0	3.762935	0	0	0.138146
Chlorine	0	0	0	0	0	4.635455	5.688361
EDC	0	0	0	0.079022	1.220215	0.231773	0.014221
VCM	0	0	0	0.079022	1.635087	0.463545	0.013525
TCE	1.980198	1	0	0.079022	0.144698	0.046355	0.043956
HCl	0	0	9.36E-01	0	0	0.463545	0.101792
SO <sub>2</sub>	0	0	1.06E+00	0	0	1.158864	0
CO <sub>2</sub>	0.019802	0	0	0	0	0.000464	0

## Appendix F Keyword input file for the VCM plant.

### Keyword Input File of ProII Program

```

$ Generated by PRO/II Keyword Generation System <version 5.61>
$ Generated on: Thu Mar 25 17:42:57 2004
TITLE DATE=09/23/03
  DIMENSION ENGLISH, TEMP=C, PRES=PSIG
  SEQUENCE SIMSCI
COMPONENT DATA
  LIBID 1,ETHYLENE/2,CL2/3,EDC/4,CCL4/5,CHCL3/6,CH3CL/7,CH4/ &
    8,DCLMETHN/9,CO/10,CO2/11,C2CL4/12,C2CL6/13,C2HCL3/14,C2HCL5/ &
    15,C2H2/16,12DCLETT/17,11DCLETE/18,12DCLETC/19,C2H2CL4/ &
    20,H2C2CL4/21,VCM/22,112TCLET/23,111TCLET/24,11DCLETH/ &
    25,C2HCL3O/26,VAC/27,CLETHANE/28,PROPDLEN/29,PROPENE/ &
    30,2CL13BD/31,13BUTD/32,BENZENE/33,HCL/34,O2/35,N2/36,H2O/ &
    37,TCLETHLN/38,H2
THERMODYNAMIC DATA
  METHOD SYSTEM=SRK, KVAL(VLE)=SRKM, DENSITY(L)=RCK1, SET=2, DEFAULT
  KVAL(VLE)
  SRKM 3,4,0.017072,0.147482,8.7493,-40.8568,0,0,1,1
  SRKM 3,5,0.097254,-0.010004,-29.4815,2.9565,0,0,1,1
  SRKM 3,13,-0.045421,0.04796,24.2198,-6.5592,0,0,1,1
  SRKM 3,21,0.047535,-0.02972,-6.5876,11.4526,0,0,1,1
  SRKM 3,24,0,0.000433,0,-4.117,0,0,1,1
  SRKM 3,32,0.014733,0.0399946,-5.0258,-13.92,0,0,1,1
  SRKM 3,33,-0.093415,-0.095866,16.8146,11.1944,0,0,0.965,0.916
  SRKM 4,5,0.019164,0.004298,-3.2167,0.6711,0,0,1.17385,0.07978
  SRKM 4,8,0.072803,-0.146358,-15.0106,52.9615,0,0,1.44081, &
    0.10411
  SRKM 4,32,-0.004987,0.007738,3.3921,-0.3973,0,0,1,1
  SRKM 4,36,0.4393,-0.1206,0,0,0,1,1
  SRKM 5,16,0.00293,-4.7128E-5,-0.17605,0.39345,0,0,1,1
  SRKM 5,24,0.051741,-0.061022,-18.7303,18.4166,0,0,1,1
  SRKM 5,32,-0.089119,-0.031971,21.2937,4.1652,0,0,1.14492, &
    1.17331
  SRKM 5,36,0.2703,-0.0641,0,0,0,1,1
  SRKM 8,13,0.005434,-0.018618,-0.339,5.0332,0,0,1,1
  SRKM 16,36,0.2255,-0.079,0,0,0,1,1
  SRKM 21,33,-0.008752,0.011038,1.789,-4.3071,0,0,1.1053,0.93789
  SRKM 22,36,0.1917,-0.1251,0,0,0,1,1
  SRKM 24,36,0.2429,-0.1171,0,0,0,1,1
  METHOD SYSTEM=SRK, DENSITY(L)=RCK1, SET=3
  WATER DECANT=ON, SOLUBILITY=SIMSCI, PROPERTY=SATURATED
STREAM DATA
  PROPERTY STREAM=OXYC, TEMPERATURE=310, PRESSURE=57.823, PHASE=M, &
    RATE(M)=212.025, COMPOSITION(M)=1,0.012812/3,0.461726/ &
    22,0.025365/33,0.000258984/34,6.47461E-5/36,0.499773, &
    NORMALIZE
  PROPERTY STREAM=RAW-DIR, TEMPERATURE=30, PRESSURE=554.24, PHASE=M, &
    RATE(M)=1700, COMPOSITION(M)=1,0.5155/2,0.4845
  PROPERTY STREAM=WTR1, TEMPERATURE=30, PRESSURE=0, PHASE=M, &
    RATE(M)=5352, COMPOSITION(M)=36,100, NORMALIZE
  PROPERTY STREAM=PYROLYSIS, TEMPERATURE=426.85, PRESSURE=420.42, &
    PHASE=M, RATE(WT)=128400, COMPOSITION(M)=1,1.91E-5/2,2.48E-9/ &

```

3,0.207/6,1.39E-6/8,4.6E-8/15,0.000306/17,1.44E-6/18,7.14E-7/ &  
 21,0.395/22,1.24E-11/27,2.98E-7/30,1.72E-14/31,4.55E-8/ &  
 33,0.397/37,1.88E-9, NORMALIZE  
 PROPERTY STREAM=EDCD, TEMPERATURE=60, PRESSURE=44.088, PHASE=M, &  
 RATE(M)=849.999, COMPOSITION(M)=1,0.064796/2,0.000363/ &  
 3,0.925681/22,0.00458/33,0.00458, NORMALIZE  
 PROPERTY STREAM=RAW-OXYC, TEMPERATURE=30, PRESSURE=554.24, PHASE=M, &  
 RATE(M)=986.2, COMPOSITION(M)=1,0.2857/33,0.5714/34,0.1429  
 NAME PYROLYSIS, FROM PYROLYSIS/EDCD, From Direct Chlorination -CSTR  
 NOTES STREAM = OXYC, TEXT = do not input components--36,34,10  
 RXDATA  
 RXSET ID=DIRECT-CL  
 REACTION ID=REAC1  
 STOICHIOMETRY 1,-1/2,-1/3,1  
 KINETICS PEXP(C, LB, FT3, PSIG, HR)=0.132, ACTIVATION=0, &  
 TEXT=0  
 KORDER 1,1/2,1  
 REACTION ID=REAC2  
 STOICHIOMETRY 1,0/2,-1/3,-1/22,1/33,1  
 KINETICS PEXP(C, LB, FT3, PSIG, HR)=0.0239, ACTIVATION=0, &  
 TEXT=0  
 KORDER 1,1/2,2/3,0  
 UNIT OPERATIONS  
 STCALCULATOR UID=OXY-CAUS  
 FEED OXYC,1  
 OVHD V=OXYD  
 BTMS L=WST2  
 FOVHD(M) 1,32,1  
 FOVHD(M) 34,36,1  
 FOVHD(M) 37,37,1  
 FOVHD(M) 38,38,1  
 FBTMS(M) 33,33,1  
 OPERATION STOP=ZERO  
 CONTROLLER UID=OXY, NAME=Balance of RX2  
 SPEC STREAM=OXYC, RATE(WT, LB/H), TOTAL, WET, DIVIDE, &  
 STREAM=RAW-OXYC, RATE(WT, LB/H), TOTAL, WET, VALUE=1  
 VARY STREAM=OXYC, RATE(LBM/H)  
 CPARAMETER IPRINT, NOSTOP  
 HX UID=E2, NAME=OXYD  
 HOT FEED=OXYD, M=OXYD2  
 OPER HTEMP=25  
 FLASH UID=OXY-FLASH  
 FEED OXYD2  
 PRODUCT V=VNT2, L=EDC2  
 ISO TEMPERATURE=25, PRESSURE=60  
 MIXER UID=MIX8  
 FEED PYROLYSIS, Q1, Q2  
 PRODUCT M=EFF2  
 FLASH UID=FLS5, NAME=POST FLASH1  
 FEED EFF2  
 PRODUCT V=VF5, L=LF5  
 ISO TEMPERATURE=160, PRESSURE=165  
 SPLITTER UID=SPL3, NAME=quench split  
 FEED LF5  
 PRODUCT M=Q1, M=QSP  
 OPERATION OPTION=FULL  
 SPEC STREAM=QSP, RATE(LBM/H), TOTAL, WET, VALUE=2000

HX UID=E5  
 HOT FEED=VF5, M=VF51  
 OPER HTEMP=90  
 FLASH UID=FLS6  
 FEED VF51  
 PRODUCT V=VF6, L=Q2  
 ISO TEMPERATURE=90, PRESSURE=150  
 HX UID=E3  
 HOT FEED=VF6, M=VF61  
 OPER HTEMP=25  
 FLASH UID=FLS7, NAME=POST FLASH2  
 FEED VF61  
 PRODUCT V=VF7, L=LF7  
 ISO TEMPERATURE=25, PRESSURE=140  
 COLUMN UID=COL3, NAME=HCL COLUMN  
 PARAMETER TRAY=42,CHEMDIST=25  
 FEED VF7,18/LF7,22  
 PRODUCT OVHD(M)=TOP3,1000, BTMS(M)=BTM3, SUPERSEDE=ON  
 CONDENSER TYPE=PART, TEST=-31  
 DUTY 1,1/2,42  
 PSPEC PTOP=135, DPCOLUMN=10  
 PRINT PROPTABLE=PART  
 ESTIMATE MODEL=CONVENTIONAL. RRATIO(L)=2.5, CTEMP=-31, RTEMP=90  
 TEMPERATURE 1,-31/6,-31/9,-25/11,0/13,20/17,20/24,22/27,40/ &  
 35,78/40,80/42,90  
 SPEC STREAM=TOP3,PPM(WT), COMP=21,WET, VALUE=100  
 SPEC STREAM=BTM3,PPM(WT), COMP=33,WET, VALUE=5  
 VARY DUTY=1,2  
 VLLECHECK CHECK=OFF  
 REBOILER TYPE=KETTLE  
 METHOD SET=2  
 COLUMN UID=COL4, NAME=VC COL  
 PARAMETER TRAY=20,CHEMDIST=100  
 FEED BTM3,7  
 PRODUCT OVHD(M)=TOP4,2000, BTMS(M)=BTM4, SUPERSEDE=ON  
 CONDENSER TYPE=BUBB  
 DUTY 1,1/2,20  
 PSPEC PTOP=65, DPCOLUMN=10  
 PRINT PROPTABLE=PART  
 ESTIMATE MODEL=CONVENTIONAL. RRATIO(L)=2.5  
 TEMPERATURE 17,140  
 SPEC RRATIO(MO), PHASE=L, VALUE=0.45  
 SPEC TRAY=17, TEMPERATURE(C), VALUE=140  
 VARY DUTY=1,2  
 VLLECHECK CHECK=OFF  
 REBOILER TYPE=KETTLE  
 METHOD SET=2  
 CONTROLLER UID=VCM-PRO, NAME=VCM capacity  
 SPEC STREAM=TOP4, RATE(WT,TS/D),TOTAL,WET, VALUE=821.9  
 VARY STREAM=PYROLYSIS, RATE(LBM/H)  
 CPARAMETER IPRINT, NOSTOP, ITER=50  
 HX UID=E1. NAME=EDCD  
 HOT FEED=EDCD, M=EDCD2  
 OPER HTEMP=25  
 CONTROLLER UID=DIR, NAME=Balance of RX1  
 SPEC STREAM=EDCD, RATE(WT,LB/H),TOTAL,WET, DIVIDE, &  
 STREAM=RAW-DIR, RATE(WT,LB/H),TOTAL,WET, VALUE=1

VARY STREAM=EDCD, RATE(LBM/H)  
 CPARAMETER IPRINT, NOSTOP  
 FLASH UID=DC-FLASH, NAME=D-COL OV FLS  
 FEED EDCD2  
 PRODUCT V=VNT1, L=EDCE  
 ISO TEMPERATURE=25, PRESSURE=13  
 STCALCULATOR UID=DC-CAUS, NAME=caustic wash  
 FEED EDCE,1  
 OVHD L=EDC1  
 BTMS L=WST1  
 FOVHD(M) 1,1,1  
 FOVHD(M) 3,32,1  
 FOVHD(M) 34,36,1  
 FOVHD(M) 37,37,1  
 FOVHD(M) 38,38,1  
 FBTMS(M) 2,2,1  
 FBTMS(M) 33,33,1  
 OPERATION STOP=ZERO  
 FLASH UID=FLS3, NAME=Saturator  
 NOTES TEXT = why VNT3 = n/a  
 FEED EDC1,EDC2,WTR1  
 PRODUCT V=VNT3, L=EDC4, W=WTR2  
 ADIABATIC DP=1  
 METHOD SET=3  
 MIXER UID=MIX6, NAME=EDC FD MIX  
 FEED EDC4,BTM4  
 PRODUCT M=EDC5  
 COLUMN UID=COL1, NAME=EDC LT COL  
 PARAMETER TRAY=17,CHEMDIST=50 DAMPING=0.7  
 FEED EDC5,2,SEPARATE  
 PRODUCT OVHD(M)=TOP1,15, BTMS(M)=BTM1, SUPERSEDE=ON  
 CONDENSER TYPE=PART  
 DUTY 1,1/2,17  
 PSPEC PTOP=185, DPCOLUMN=22  
 PRINT PROPTABLE=PART  
 ESTIMATE MODEL=CHEM, RRATIO(L)=3  
 SPEC STREAM=TOP1, RATE(LBM/H), COMP=3,WET, DIVIDE, STREAM=EDC5, &  
 RATE(LBM/H), COMP=3,WET, VALUE=0.001  
 SPEC RRATIO(MO), PHASE=L, VALUE=2.1  
 VARY DUTY=1,2  
 VLLECHECK CHECK=OFF  
 METHOD SET=2  
 MIXER UID=MIX7, NAME=HVY FD MIX  
 FEED BTM1,VAPP  
 PRODUCT M=HVYF  
 COLUMN UID=COL2, NAME=HVY COL  
 PARAMETER TRAY=30,IO  
 FEED HVYF,17/QSP,29  
 PRODUCT OVHD(M)=TOP2, BTMS(M)=BTM2,30, SUPERSEDE=ON  
 CONDENSER TYPE=BUBB  
 DUTY 1,1/2,30  
 PSPEC PTOP=60, DPCOLUMN=15  
 PRINT PROPTABLE=PART  
 SPEC RRATIO, VALUE=0.6, RTOLER=0.0001  
 SPEC STREAM=BTM2, RATE(LBM/H), COMP=3,WET, DIVIDE, STREAM=HVYF, &  
 RATE(LBM/H), COMP=3,WET, VALUE=0.03, RTOLER=0.0001  
 VARY DUTY=1,2

```

REBOILER TYPE=KETTLE
METHOD SET=2
HX UID=E4
HOT FEED=TOP2, M=TOP21
OPER HTEMP=200
OPTIMIZER UID=OP3
VARY ID=OPT3VARY1, COLUMN=COL3, FTRAY(1), MINI=15, MAXI=30
VARY ID=OPT3VARY2, COLUMN=COL3, FTRAY(2), MINI=15, MAXI=40
OBJECTIVE COLUMN=COL3, DUTY(2,BTU/HR), MINIMIZE
OPTIMIZER UID=OP4
VARY ID=OPT4VARY1, COLUMN=COL4, FTRAY(1), MINI=3, MAXI=19
OBJECTIVE COLUMN=COL4, DUTY(2,BTU/HR), MINIMIZE
FLASH UID=FLS4, NAME=PYRO FD FLSH
FEED TOP21
PRODUCT V=PYRF, L=VAPP
TPSPEC TESTIMATE=200, PRESSURE=200
SPEC STREAM=VAPP, RATE(WT,LB/H),TOTAL,WET, VALUE=10000
OPTIMIZER UID=OP2
VARY ID=OPT4VARY2, COLUMN=COL2, FTRAY(1), MINI=15, MAXI=20
VARY ID=OPT4VARY3, COLUMN=COL2, FTRAY(2), MINI=25, MAXI=29
OBJECTIVE COLUMN=COL2, DUTY(2,BTU/HR), MINIMIZE
CONTROLLER UID=CN3
SPEC STREAM=PYRF, RATE(WT,LB/H),TOTAL,WET, DIVIDE, &
STREAM=PYROLYSIS, RATE(WT,LB/H),TOTAL,WET, VALUE=1
VARY STREAM=EDCD, RATE(LBM/H)
CPARAMETER IPRINT, NOSTOP, ITER=100
MIXER UID=M1
FEED VNT1,VNT3,VNT2,BTM2, TOP1
PRODUCT M=W-VOC
MIXER UID=M2
FEED WST1,WST2,WTR2
PRODUCT M=W-WATER
END

```

### Keyword Input File of GAMS Program

```

sets
i year /i1*i20/
s scenario /s1*s1000/

parameters
PE(s) Purchased Equipment(US$)
FCI(s) Fixed Capital Investment(US$)
Ep(i,s) Ethylene Price(dollar per ton)
VCMp(i,s) Vinyl Chloride Price(dollar per ton)
D_VCM(i,s) Demand of VCM in Thailand(ton)
Mar(i,s) Annual-compounding discount rate or minimum acceptable rate of return
Env_imp(s) Environmental Impact Unit (EIU per ton of VCM)
Fac_EP(s) Ethylene Consumption (ton Ethylene per ton of VCM)

Fac_Uilities(s) Utilities Consumption (US$ per ton of VCM)
Lab_Cost(s) Labor Cost (US$ per year)
Oyear(i) year
MACRS(i) Using 5-y MACRS
*****

```



```

*****
*****
Ethylene(s)   Waste production of Ethylene (kg per ton VCM production)
Chlorine(s)   Waste production of Chlorine (kg per ton VCM production)
EDC(s)        Waste production of EDC (kg per ton VCM production)
VCM(s)        Waste production of VCM (kg per ton VCM production)
TCE(s)        Waste production of TCE (kg per ton VCM production)
HCl(s)        Waste production of HCl (kg per ton VCM production)
SO2(s)        Waste production of SO2 (kg per ton VCM production)
CO2(s)        Waste production of CO2 (kg per ton VCM production)
GWP_TCE(s)
GWP_CO2(s)
ODP_TCE(s)
AP_SO2(s)
AP_HCl(s)
PCOP_Ethylene(s)
PCOP_3c(s)
HTPIaTTP_EDC(s)
HTPIaTTP_VCM(s)
HTPIaTTP_TCE(s)
HTPE_chlorine(s)
HTPE_EDC(s)
HTPE_VCM(s)
HTPE_TCE(s)
HTPE_HCl(s)
HTPE_SO2(s)
HTPE_CO2(s)
ATP_Ethylene(s)
ATP_Chlorine(s)
ATP_EDC(s)
ATP_VCM(s)
ATP_TCE(s)
ATP_HCl(s)
;
CO2(s) = normal(224.165,224.165*0.1);
SO2(s) = normal(0.5442,0.5442*0.1);
Ethylene(s) = normal(0,0);
Chlorine(s) = normal(0,0);
EDC(s) = normal(0,0);
VCM(s) = normal(0,0);
TCE(s) = normal(0,0);
HCl(s) = normal(0,0);
*required user input*****

GWP_TCE(s) = normal(1.9802,1.8902*0.1);
GWP_CO2(s) = normal(0.0198,0.0198*0.1);
ODP_TCE(s) = normal(1,0.1);
AP_SO2(s) = normal(1.06,1.06*0.1);
AP_HCl(s) = normal(0.936,0.936*0.1);
PCOP_Ethylene(s) = normal(3.7629,3.7629*0.1);
PCOP_3c(s) = normal(0.0790,0.0790*0.1);
HTPIaTTP_EDC(s) = normal(1.2202,1.2202*0.1);
HTPIaTTP_VCM(s) = normal(1.6351,1.6351*0.1);
HTPIaTTP_TCE(s) = normal(0.1447,0.1447*0.1);
HTPE_chlorine(s) = normal(4.6354,4.6354*0.1);
HTPE_EDC(s) = normal(0.2318,0.2318*0.1);
HTPE_VCM(s) = normal(0.4635,0.4635*0.1);

```

```

HTPE_TCE(s) = normal(0.0464,0.0464*0.1);
HTPE_HCl(s) = normal(0.4635,0.4635*0.1);
HTPE_SO2(s) = normal(1.1589,1.1589*0.1);
HTPE_CO2(s) = normal(0.0005,0.0005*0.1);
ATP_Ethylene(s) = normal(0.1381,0.1381*0.1);
ATP_Chlorine(s) = normal(5.6884,5.6884*0.1);
ATP_EDC(s) = normal(0.0142,0.0142*0.1);
ATP_VCM(s) = normal(0.0135,0.0135*0.1);
ATP_TCE(s) = normal(0.0440,0.0440*0.1);
ATP_HCl(s) = normal(0.1018,0.1080*0.1);

Env_Imp(s) = GWP_TCE(s)*TCE(s)+GWP_CO2(s)*CO2(s)
+ODP_TCE(s)*TCE(s)+AP_SO2(s)*SO2(s)+AP_HCl(s)*HCl(s)
+PCOP_Ethylene(s)*Ethylene(s)
+PCOP_3c(s)*(EDC(s)+VCM(s)+TCE(s))
+HTPlatTP_EDC(s)*2*EDC(s)+HTPlatTP_VCM(s)*2*VCM(s)
+HTPlatTP_TCE(s)*2*TCE(s)+HTPE_chlorine(s)*Chlorine(s)
+HTPE_EDC(s)*EDC(s)+HTPE_VCM(s)*VCM(s)+HTPE_TCE(s)*TCE(s)
+HTPE_HCl(s)*HCl(s)+HTPE_SO2(s)*SO2(s)+HTPE_CO2(s)*CO2(s)
+ATP_Ethylene(s)*Ethylene(s)+ATP_Chlorine(s)*Chlorine(s)
+ATP_EDC(s)*EDC(s)+ATP_VCM(s)*VCM(s)
+ATP_TCE(s)*TCE(s)+ATP_HCl(s)*HCl(s) ;
*****
*****
*****
Lab_Cost(s) = normal(55638,55638*0.1);
*Cap 300000 ton/y*****
*Lab_Cost(s) = normal(57800,57800*0.1);
*Cap 400000 ton/y*****
*Lab_Cost(s) = normal(59477,59477*0.1);
*Cap 500000 ton/y*****

Fac_EP(s)= 0.4750;
*required user input*****

Fac_Uilities(s)= normal(52.5,52.5*0.1);
*required user input*****

PE(s)= normal(5584056,5584056*0.3);
*required user input*****

Oyear('i1') = 1 ;
Oyear('i2') = 2 ;
Oyear('i3') = 3 ;
Oyear('i4') = 4 ;
Oyear('i5') = 5 ;
Oyear('i6') = 6 ;
Oyear('i7') = 7 ;
Oyear('i8') = 8 ;
Oyear('i9') = 9 ;
Oyear('i10') = 10 ;
Oyear('i11') = 11 ;
Oyear('i12') = 12 ;
Oyear('i13') = 13 ;

```

Oyear('i14') = 14 ;  
 Oyear('i15') = 15 ;  
 Oyear('i16') = 16 ;  
 Oyear('i17') = 17 ;  
 Oyear('i18') = 18 ;  
 Oyear('i19') = 19 ;  
 Oyear('i20') = 20 ;

MACRS('i1') = 0.2 ;  
 MACRS('i2') = 0.32 ;  
 MACRS('i3') = 0.192 ;  
 MACRS('i4') = 0.1152 ;  
 MACRS('i5') = 0.1152 ;  
 MACRS('i6') = 0.0576 ;  
 MACRS('i7') = 0.0 ;  
 MACRS('i8') = 0.0 ;  
 MACRS('i9') = 0.0 ;  
 MACRS('i10') = 0.0 ;  
 MACRS('i11') = 0.0 ;  
 MACRS('i12') = 0.0 ;  
 MACRS('i13') = 0.0 ;  
 MACRS('i14') = 0.0 ;  
 MACRS('i15') = 0.0 ;  
 MACRS('i16') = 0.0 ;  
 MACRS('i17') = 0.0 ;  
 MACRS('i18') = 0.0 ;  
 MACRS('i19') = 0.0 ;  
 MACRS('i20') = 0.0 ;

Mar(i,s)= uniform(0.08,0.16) ;

\*Using Mar in this range because new capacity

\*with established corporate market position

\*Ref:Table 8-1, P.322

Ep('i1',s)= normal(-4.8568\*2007+10170,107.38);  
 Ep('i2',s)= normal(-4.8568\*2008+10170,107.38);  
 Ep('i3',s)= normal(-4.8568\*2009+10170,107.38);  
 Ep('i4',s)= normal(-4.8568\*2010+10170,107.38);  
 Ep('i5',s)= normal(-4.8568\*2011+10170,107.38);  
 Ep('i6',s)= normal(-4.8568\*2012+10170,107.38);  
 Ep('i7',s)= normal(-4.8568\*2013+10170,107.38) ;  
 Ep('i8',s)= normal(-4.8568\*2014+10170,107.38) ;  
 Ep('i9',s)= normal(-4.8568\*2015+10170,107.38) ;  
 Ep('i10',s)= normal(-4.8568\*2016+10170,107.38) ;  
 Ep('i11',s)= normal(-4.8568\*2017+10170,107.38) ;  
 Ep('i12',s)= normal(-4.8568\*2018+10170,107.38) ;  
 Ep('i13',s)= normal(-4.8568\*2019+10170,107.38) ;  
 Ep('i14',s)= normal(-4.8568\*2020+10170,107.38) ;  
 Ep('i15',s)= normal(-4.8568\*2021+10170,107.38) ;  
 Ep('i16',s)= normal(-4.8568\*2022+10170,107.38) ;  
 Ep('i17',s)= normal(-4.8568\*2023+10170,107.38) ;  
 Ep('i18',s)= normal(-4.8568\*2024+10170,107.38) ;  
 Ep('i19',s)= normal(-4.8568\*2025+10170,107.38) ;  
 Ep('i20',s)= normal(-4.8568\*2026+10170,107.38) ;

VCMP('i1',s)= normal(1.3395\*2007-2193.9,114.06) ;

VCMP('i2',s)= normal(1.3395\*2008-2193.9,114.06) ;

VCMP('i3',s)= normal(1.3395\*2009-2193.9,114.06) ;  
 VCMP('i4',s)= normal(1.3395\*2010-2193.9,114.06) ;  
 VCMP('i5',s)= normal(1.3395\*2011-2193.9,114.06) ;  
 VCMP('i6',s)= normal(1.3395\*2012-2193.9,114.06) ;  
 VCMP('i7',s)= normal(1.3395\*2013-2193.9,114.06) ;  
 VCMP('i8',s)= normal(1.3395\*2014-2193.9,114.06) ;  
 VCMP('i9',s)= normal(1.3395\*2015-2193.9,114.06) ;  
 VCMP('i10',s)= normal(1.3395\*2016-2193.9,114.06) ;  
 VCMP('i11',s)= normal(1.3395\*2017-2193.9,114.06) ;  
 VCMP('i12',s)= normal(1.3395\*2018-2193.9,114.06) ;  
 VCMP('i13',s)= normal(1.3395\*2019-2193.9,114.06) ;  
 VCMP('i14',s)= normal(1.3395\*2020-2193.9,114.06) ;  
 VCMP('i15',s)= normal(1.3395\*2021-2193.9,114.06) ;  
 VCMP('i16',s)= normal(1.3395\*2022-2193.9,114.06) ;  
 VCMP('i17',s)= normal(1.3395\*2023-2193.9,114.06) ;  
 VCMP('i18',s)= normal(1.3395\*2024-2193.9,114.06) ;  
 VCMP('i19',s)= normal(1.3395\*2025-2193.9,114.06) ;  
 VCMP('i20',s)= normal(1.3395\*2026-2193.9,114.06) ;

D\_VCM('i1',s)= normal(41\*2007\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i2',s)= normal(41\*2008\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i3',s)= normal(41\*2009\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i4',s)= normal(41\*2010\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i5',s)= normal(41\*2011\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i6',s)= normal(41\*2012\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i7',s)= normal(41\*2013\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i8',s)= normal(41\*2014\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i9',s)= normal(41\*2015\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i10',s)= normal(41\*2016\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i11',s)= normal(41\*2017\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i12',s)= normal(41\*2018\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i13',s)= normal(41\*2019\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i14',s)= normal(41\*2010\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i15',s)= normal(41\*2021\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i16',s)= normal(41\*2022\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i17',s)= normal(41\*2023\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i18',s)= normal(41\*2024\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i19',s)= normal(41\*2025\*1000-82027\*1000,14.76\*1000) ;  
 D\_VCM('i20',s)= normal(41\*2026\*1000-82027\*1000,14.76\*1000) ;

#### Scalars

Land\_Rent Land Rent in Map Ta Phut Industrial Estate Per Year /176282/  
 CapVCM Capacity of VCM plant 300000 ton per year /300000/  
 \*CapVCM Capacity of VCM plant 400000 ton per year /400000/  
 \*CapVCM Capacity of VCM plant 500000 ton per year /500000/  
 \*required user choose one capacity of plant-----

#### Parameters

LC(S) Laborating\_Charges  
 OpeS(s) Operating\_supplies  
 OS(s) Operation\_Supervision  
 MR(s) Maintenance\_and\_repairs  
 FC(s) Fixed\_Charges

;  
 FCI(s)= (PE(s)\*1.10)\*(1+2.6+1.44) ;  
 OS(s) = Lab\_Cost(s)\*0.15 ;  
 MR(s) = 0.06\*FCI(s) ;

$OpeS(s) = 0.06 * 0.15 * FCI(s) ;$   
 $LC(s) = Lab\_Cost(s) * 0.15 ;$   
 $FC(s) = 0.03 * FCI(s) + Land\_Rent ;$

#### Variables

Tax(i,s)  
 AP(i,s)            Annual production capacity(ton per year)  
 RMC(i,s)           Raw\_Material\_Cost  
 PV(i,s)            Product\_Value  
 VC(i,s)            Variable\_Cost  
 POC(i,s)           Plant\_Overhead\_Costs  
 MC(i,s)            Manufacturing\_Cost  
 Co(i,s)            Total\_Product\_Cost  
 GE(i,s)            General\_Expense  
 AGP(i,s)           Annual\_Gross\_Profit  
 Ann\_Net\_Profit(i,s) Annual\_Net\_Profit  
 TACF(i,s)          Total\_Annual\_Cash\_Flow  
 PWACF(i,s)        Present\_Worth\_of\_ACF  
 WC(s)            Working\_Capital  
 TCI(s)            Total\_Capital\_Investment  
 TACF\_Y0(s)        TotalAnnualCashFlow\_Y0  
 NPW(s)            Net\_Present\_Worth  
 AVE\_NPW           Average\_NPW  
 Ann\_EIU(i,s)       Annual\_EIU  
 AVE\_EIU           Average\_EIU  
 Tot\_EIU(s)        Tot\_EIU  
 Tot\_AGP(s)        ;

#### Parameters

net\_HCl(s)        ton per ton VCM  
 net\_Cl2(s)        ton per ton VCM  
 net\_O2(s)        ton per ton VCM  
 P\_HCl(s)         price of HCl (\$ per ton)  
 P\_Cl2(s)         price of Cl2 (\$ per ton)  
 P\_O2(s)         price of O2 (\$ per ton);

net\_HCl(s) =0.3005 ;  
 \*required user input\*\*\*\*\*  
 net\_Cl2(s) =0.8521 ;  
 \*required user input\*\*\*\*\*  
 net\_O2(s) =0.0659;  
 \*required user input\*\*\*\*\*  
 P\_HCl(s) = normal(273,73.3);  
 P\_Cl2(s) = normal(210.4,69.7);  
 P\_O2(s) = normal(40,4);

#### Equations

Working\_Capital(s)  
 Total\_Capital\_Investment(s)  
 TotalAnnualCashFlow\_Y0(s)  
 Net\_Present\_Worth(s)  
 Average\_NPW  
 Total\_EIU(s)  
 Average\_EIU  
 Total\_AGP(s)  
 ;

\*Financial =====

Working\_Capital(s) .. WC(s) =e= PE(s)\*1.10\*0.89;  
 Total\_Capital\_Investment(s) .. TCI(s) =e= FCI(s)+WC(s);

\*year0++++  
 TotalAnnualCashFlow\_Y0(s) ..  
 TACF\_Y0(s) =e= (Land\_Rent+FCI(s)+WC(s))\*(-1) ;

\*Year1-20\*\*\*\*\*

loop(i,  
 AP.l(i,s) = CapVCM\$(D\_VCM(i,s)>CapVCM)  
 +D\_VCM(i,s)\$(D\_VCM(i,s)<CapVCM)  
 +D\_VCM(i,s)\$(D\_VCM(i,s)=CapVCM);

RMC.l(i,s) = Ep(i,s)\*AP.l(i,s)\*Fac\_EP(s)  
 +(net\_Cl2(s)\*P\_Cl2(s)+net\_O2(s)\*P\_O2(s))\*AP.l(i,s);

PV.l(i,s) = net\_HCl(s)\*P\_HCl(s)\*AP.l(i,s)+AP.l(i,s)\*VCMp(i,s) );

loop(i,  
 VC.l(i,s) = RMC.l(i,s)+ Lab\_Cost(s) + Fac\_Uilities(s)\*AP.l(i,s)  
 + OS(s) + MR(s) + OpeS(s) + LC(s) );

loop(i,  
 POC.l(i,s) = 0.6\*(Lab\_Cost(s) + OS(s) + MR(s)) ;  
 MC.l(i,s) = VC.l(i,s)+ FC(s) + POC.l(i,s) ;  
 Co.l(i,s) = (MC.l(i,s)+ 0.2\*(Lab\_Cost(s)+OS(s)+MR(s)))  
 /(1-0.01-0.05-0.04) ;  
 GE.l(i,s)= 0.2\*(Lab\_Cost(s) + OS(s)  
 + MR(s))+0.05\*Co.l(i,s)+0.04\*Co.l(i,s);  
 AGP.l(i,s) = PV.l(i,s) - Co.l(i,s)- MACRS(i)\*FCI(s) ;  
 Tax.l(i,s)= 0.3\$(AGP.l(i,s)>0)+0\$(AGP.l(i,s)<0) ;  
 Ann\_Net\_Profit.l(i,s)= AGP.l(i,s)\*(1-tax.l(i,s)) ;  
 TACF.l(i,s) = Ann\_Net\_Profit.l(i,s)+ MACRS(i)\*FCI(s) ;  
 PWACF.l(i,s) = TACF.l(i,s)\*(1+Mar(i,s))\*(-Oyear(i)) ;

\*Environmental Impact

Index=====

Ann\_EIU.l(i,s) = AP.l(i,s)\*Env\_Imp(s) );

\*All

Years=====

Net\_Present\_Worth(s) ..NPW(s) =e= TACF\_Y0(s)+ sum(i,PWACF.l(i,s)) ;

Total\_EIU(s).. sum(i, Ann\_EIU.l(i,s))/sum(i,AP.l(i,s)) =e= Tot\_EIU(s) ;

Average\_NPW ..sum(s, NPW(s))/1000 =e= AVE\_NPW ;

Average\_EIU .. sum(s, Tot\_EIU(s))/1000 =e= AVE\_EIU ;

Total\_AGP(s) .. sum(i, AGP.l(i,s)) =e= Tot\_AGP(s);

```
Model All_NPW /all/
```

```
Solve All_NPW using lp maximizing AVE_NPW;
```

```
Display NPW.l, AVE_NPW.l, Tot_EIU.l, AVE_EIU.l, PWACF.l, AP.l, TACF_Y0.l, tax.l, Mar, MACRS  
;
```

```
File pilot_result /C:\result_GAM\result_DST.excel/;
```

```
  pilot_result.pc=6 ;
```

```
put pilot_result;
```

```
put /;
```

```
put "Scenarios", "NPW", "AVE_NPW", "Tot_EIU", "AVE_EIU", "TCI", "Total_AGP" /;
```

```
loop (s, put s.tl, NPW.l(s):10:4, AVE_NPW.l:10:4, Tot_EIU.l(s):10:4, AVE_EIU.l:10:4,
```

```
TCI.l(s):10:4, Tot_AGP.l(s):10:4/);
```

```
*
```

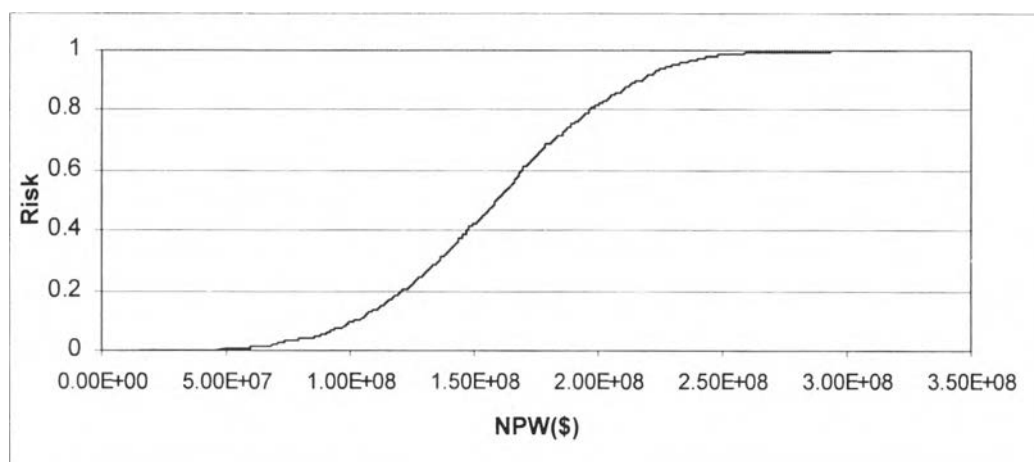
## Appendix G Reference data of VCM plant from Dr. Thevarak Rochanapruk.

### Input Data to GAMS Program

**Table G1** Reference data from Thai Plastics and Chemicals Co., Ltd.

Data	Value
Utility cost	25 \$/ton of VCM
Land rent	20,000,000 \$/year
Labor cost	8,000,000 \$/year
Purchased equipment cost	150,000,000 \$ at a capacity of 250,000 tons/year
Working capital cost	35,000,000 \$
Indirect cost	70,000,000 \$
Total cost	255,000,000 \$
Ethylene consumption	0.250 ton Ethylene/ton VCM
Oxygen consumption	0.190 ton Oxygen/ton VCM
Chlorine consumption	0.005 ton Chlorine/ton VCM
Price of chlorine	210 \$/ton
Price of oxygen	150 \$/ton

### Results



**Figure G1** Financial risk curve.

From the data, financial risk curve is shown in Figure G1 with the expected net present worth of \$159,081,000 and the standard deviation of \$44,237,647



## CURRICULUM VITAE

**Name:** Ms. Mayurachat Ounjitti

**Date of Birth:** May 5, 1981

**Nationality:** Thai

**University Education:**

1998-2002 Bachelor Degree of Science in Industrial Chemistry, Faculty of Applied Science, King Mongkut's Institute of Technology North Bangkok, Bangkok, Thailand.