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APPENDICES

Appendix A Kinetic model reaction.

Table A1 Kinetic Model of Reaction

Overall Rate Equations	Unit
d(p10)/d(t) = ((-2.54*p10*A-.49*p10*B-.63*p10*B-1.09*p10*B-.89*p10*B-1.24*p10*B)+1.34*n10*C+.16*a10*C)*.01	(gmol)/s
d(n10)/d(t) = (2.54*p10*A+(-.54*n10*C-1.34*n10*C-1.34*n10*B-.8*n10*B-24.5*n10*D))*.01	(gmol)/s
d(a10)/d(t) = (24.5*n10*D+(-.16*a10*C-.06*a10*C-.06*a10*C))*.01	(gmol)/s
d(p9)/d(t) = (.49*p10*B+(-1.81*p9*A-.3*p9*B-.39*p9*B-.68*p9*B-.55*p9*B)+.54*n9*C+.16*a9*C)*.01	(gmol)/s
d(n9)/d(t) = (.54*n10*C+1.81*p9*A+(-.54*n9*C-1.27*n9*C-1.27*n9*C-24.50*n9*D))*.01	(gmol)/s
d(a9)/d(t) = (.06*a10*C+24.50*n9*D+(-.16*a9*C-.05*a9*C-.05*a9*C))*.01	(gmol)/s
d(p8)/d(t) = (.63*p10*B+(-.19*p8*B-.25*p8*B-.43*p8*B-.35*p8*B)+.47*n8*C+.16*a8*C+.3*p9*B-1.33*p8*A)*.01	(gmol)/s
d(n8)/d(t) = (1.34*n10*B+(-.47*n8*C-.09*n8*C-21.5*n8*D)+1.27*n9*C+1.33*p8*A)*.01	(gmol)/s
d(a8)/d(t) = (.06*a10*C+21.5*n8*D+(-.16*a8*C-.01*a8*C)+.05*a9*C)*.01	(gmol)/s
d(p7)/d(t) = (1.09*p10*B+.19*p8*B+(-.58*p7*A-.14*p7*B-.18*p7*B-.39*p7*B)+.39*p9*B+.2*n7*C+.16*a7*C)*.01	(gmol)/s
d(n7)/d(t) = (.8*n10*B+.09*n8*C+.58*p7*A+1.27*n9*C+(-.2*n7*C-9.03*n7*D))*.01	(gmol)/s
d(a7)/d(t) = (.01*a8*C+.05*a9*C+9.03*n7*D-.16*a7*C)*.01	(gmol)/s
d(p6)/d(t) = (.89*p10*B+.25*p8*B+.14*p7*B+.68*p9*B+(-.14*p6*B-.18*p6*B-.27*p6*B)+1.48*n6*C)*.01	(gmol)/s
d(n6)/d(t) = ((-1.48*n6*C-4.02*n6*D)+.45*a6*C)*.01	(gmol)/s
d(a6)/d(t) = (4.02*n6*D-.45*a6*C)*.01	(gmol)/s
d(p5)/d(t) = (2*1.24*p10*B+.43*p8*B+.18*p7*B+.55*p9*B+.14*p6*B+(-.12*p5*B-.15*p5*B))*.01	(gmol)/s
d(p4)/d(t) = (.89*p10*B+2*.35*p8*B+.39*p7*B+.55*p9*B+.18*p6*B+.12*p5*B)*.01	(gmol)/s
d(p3)/d(t) = (1.09*p10*B+.43*p8*B+.39*p7*B+.68*p9*B+2*.27*p6*B+.15*p5*B)*.01	(gmol)/s
d(p2)/d(t) = (.63*p10*B+.25*p8*B+.18*p7*B+.39*p9*B+.18*p6*B+.15*p5*B)*.01	(gmol)/s
d(p1)/d(t) = (.49*p10*B+.19*p8*B+.14*p7*B+.3*p9*B+.14*p6*B+.12*p5*B)*.01	(gmol)/s

Table A1 (Continue)

Correction Parameter	Unit
A = (P/21)^(-.7)*exp(45/R*(1/773-1/(T+273))) ;Dehydrocyclization reaction	-
B = (P/21)^.433*exp(55/R*(1/773-1/(T+273))) ;Hydrocracking reaction	-
C = (P/21)^.5*exp(40/R*(1/773-1/(T+273))) ;Hydrodealkylation reaction	-
D = (P/21)^0*exp(30/R*(1/773-1/(T+273))) ;Dehydrogenation reaction	-
R = 1.987*.001	(Kcal)/(gmol)(K)
Variable	**Unit**
T = Temperature	Degree Celsius
P = Pressure	bar

Appendix B Heat exchanger network design.

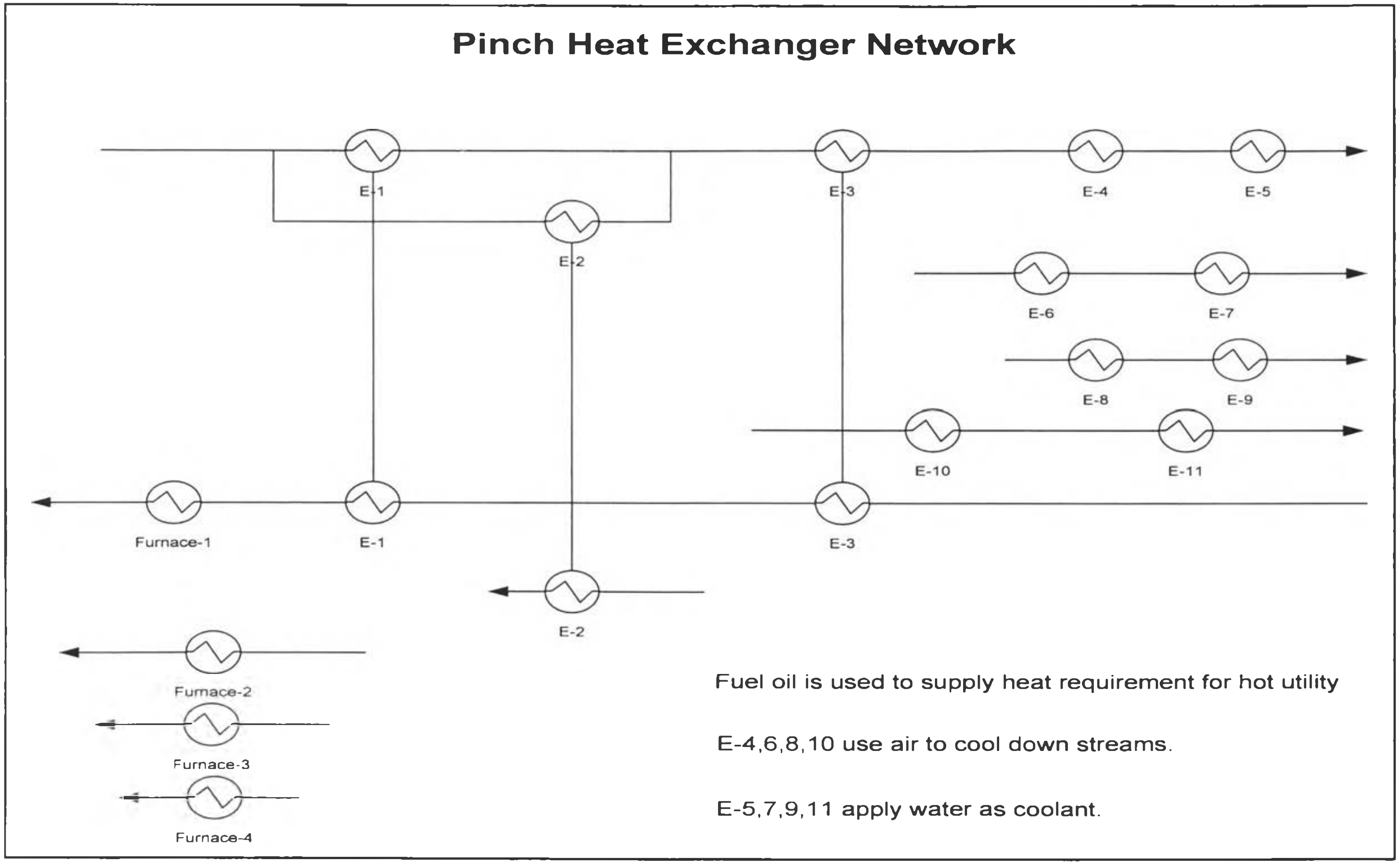

Figure B1 Pinch Heat Exchanger Network type.

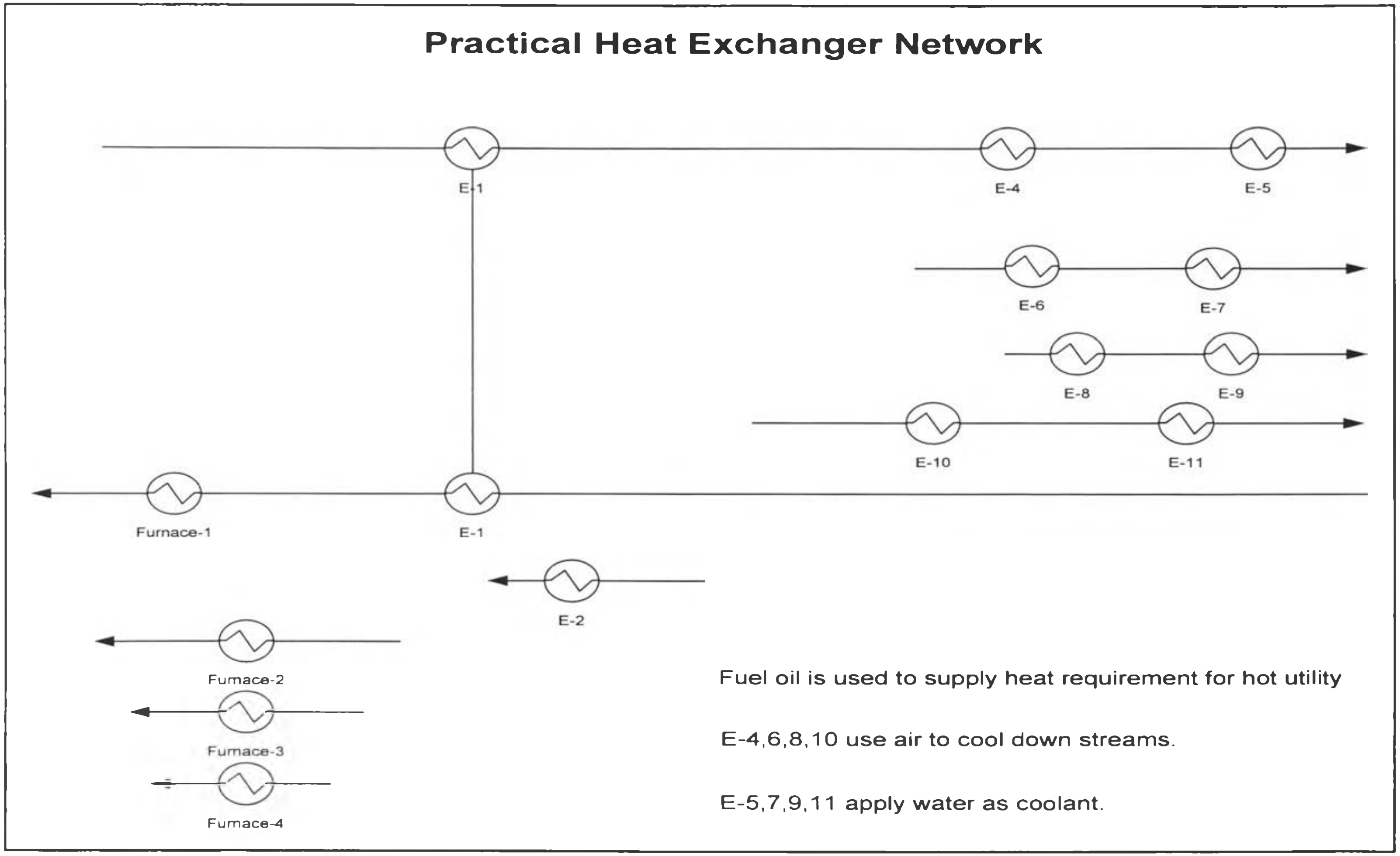

Figure B2 Practical Heat Exchanger Network type.

Appendix C Profit and environmental impact evaluation.

Table C1 Estimation of fixed-capital Investment cost

Direct costs	$
Total bar-module equipment cost, (C_{tbm}) Building, process and auxiliary service facilities and yard improvements Land Total direct cost , (C_{tdc})	C_{tbm} 13%C_{tbm} 20%C_{tbm} 2%C_{tbm} 135%C_{tbm}
Indirect costs	**$**
Engineering and supervision Construction expense and contractor fee Contingency Total Indirect cost	10%C_{tdc} 14%C_{tdc} 15%C_{tdc} 53 C_{tbm}
Fixed capital investment (C_{fix})	**$**
Direct cost + indirect cost	188%C_{tbm}
Working-capital investment	**$**
	18%C_{fix}
Total capital investment, (C_{tci})	**$**
Fixed capital + working-capital investment	221%C_{tbm}

Table C2 Estimation of gross earning and total production cost per year

Manufacturing cost, (Cmc)	\$/year
A. Direct production costs	
Raw materials	C_{raw}
Operating & direct supervisory labo-	C_{lab}
Utilities	C_u
Maintenance and repairs, (C_{mr})	$6\%C_{fix}$
operating supplies	$.75\%C_{fix}$
Laboratory charges	$15\%C_{lab}$
B. Fixed charges	
Depriciation	$17\%C_{tbm}$
Local taxes	$2.5\%C_{fix}$
Insurance	$7\%C_{fix}$
C. Plant-overhead costs	$60\%(C_{lar}+C_{mr})$
General expenses	**\$/year**
Administrative costs	$15\%(C_{lar}+C_{mc})$
Distribution and selling costs	$15\%C_{tpc}$
Research and development costs	$4\%C_{tpc}$
Financing	$3.5\%C_{tci}$
Total production cost	**\$/year**
manufacturing cost + general expenses	C_{tpc}
Gross-earnings	**\$/year**
Total income - total production cost	C_g

Measuring the process' s profit

There are many ways in profitability measuring step, even though the net present value, (NPV), is normally considered to be the simplest and easies understandable method. Hence, in this research, it is used to be the method in profit assessment. The concept of calculation are in the below equation.

$$P = \frac{S}{(1+i)^n} \tag{1}$$

where P is the present value, S is the future worth value, i is interest rate, n is the number of years.

To evaluate the net present (NPV) of each design, its cash flow was computed in each year of the projected life of the plant, fixed-capital Investment cost and gross-earnings. Then, by the interest rate (typically 15% for most company management), each cash flow was discounted to its present worth. The sum of all discounted cash flow was the net present values.

Measuring the process' s environmental impact

In this study, overall amount of hazardous substance, produced from each design, is regarded as environmental impact for each design.

To find overall environmental impact, amount of carbon dioxide and benzene are combined to be representative impact for each design. In this work, benzene was valued to have 3.5 times impact greater than carbon dioxide, due to higher concern in the carcinogenic hazardous effect. Hence, the formula of environmental impact evaluation could be derived as in equation 3.7.

$$Environmental\ impact = 3.5 * \text{benzene amonut} + \text{carbon dioxide amount} \tag{2}$$

Appendix D Coke formation and octane number.

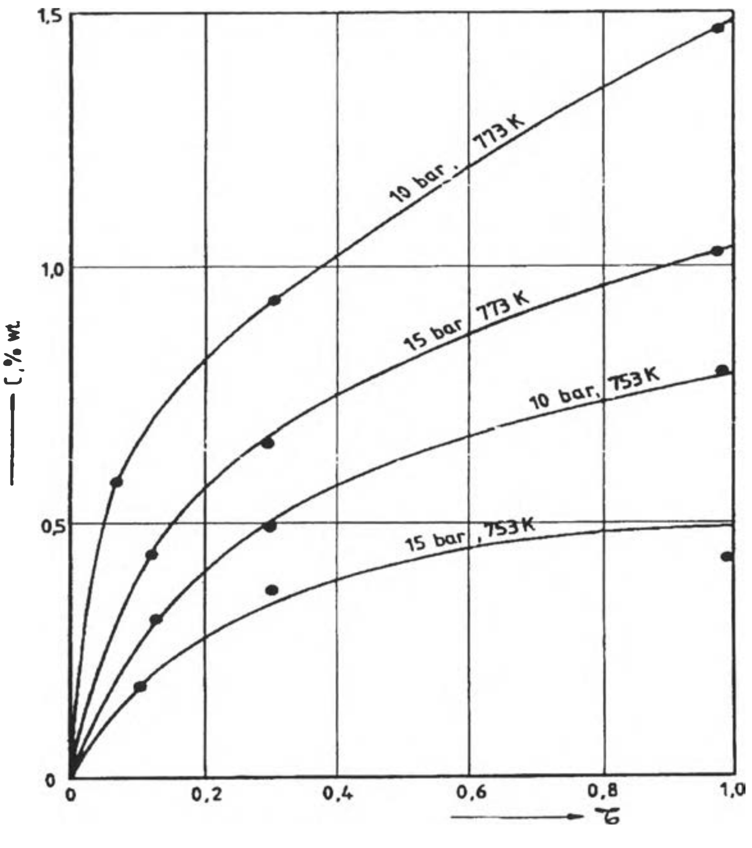

Figure D1 Coke formation (C % wt) vs. relative reaction time (τ).

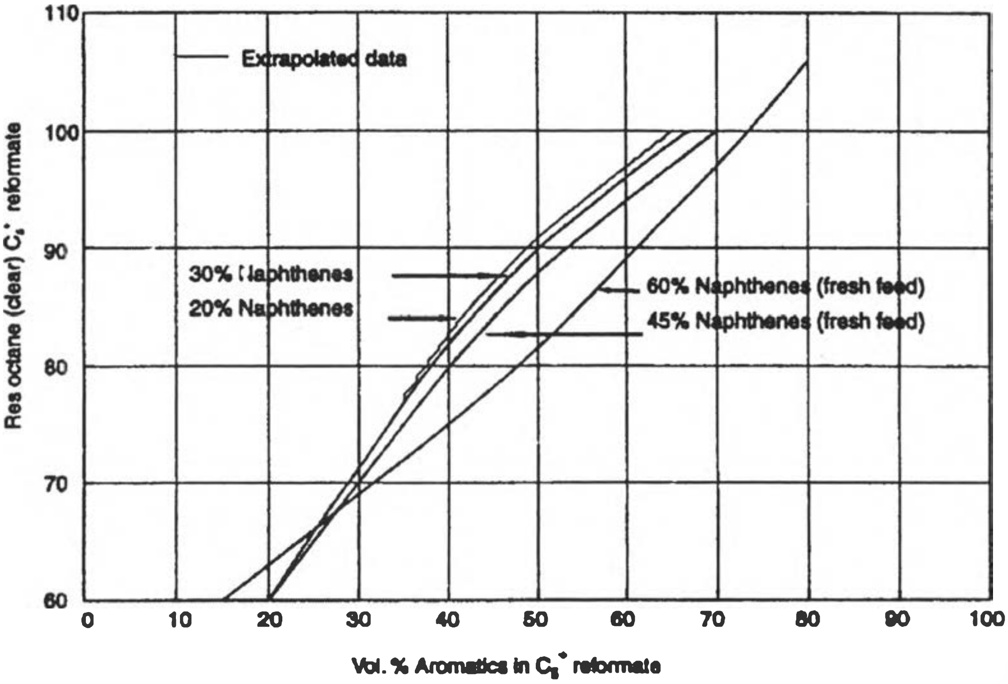

Figure D2 Octane number vs. aromatics amount of reformate.

Appendix E Chemical prices and uncertainty source.

Table E1 Raw material, Product, by-product and utilities prices in Year 1991-2003

Year	Raw Material	Product		By-Product		Plant Utility	
	Naphtha ($/bbl)	Reformate(73%aromatic) ($/bbl)	Reformate(77%aromatic) ($/bbl)	Hydrogen ($/m^3)	LPG ($/kg)	Fuel Oil ($/bbl)	Water ($/m^3)
1991	22.83	-	-	0.09	0.25	14.04	0.49
1992	20.27	-	-	0.08	0.24	13.39	0.49
1993	17.18	-	-	0.07	0.24	11.76	0.44
1994	16.36	23.69	24.74	0.06	0.24	13.14	0.44
1995	17.54	24.43	26.04	0.07	0.24	14.92	0.44
1996	20.26	25.73	26.55	0.08	0.24	16.78	0.44
1997	21.85	26.61	27.33	0.08	0.25	15.87	0.49
1998	14.77	19.27	20.09	0.06	0.28	10.63	0.60
1999	19.54	23.28	23.87	0.08	0.23	15.75	0.60
2000	28.38	34.82	35.81	0.11	0.22	24.49	0.60
2001	19.10	29.64	30.80	0.07	0.25	20.70	0.60
2002	24.93	30.12	30.92	0.10	0.30	22.38	0.60
2003	29.71	36.85	37.73	0.11	0.32	26.22	0.60

Table E2 uncertain parameters

Parameter	Distribution type	Uncertainty (%)
Reformate Demand	Normal distribution	25.53
Naphtha price	Normal distribution	19.33
Reformate(73%aromatic) price	Normal distribution	21.45
Reformate(77%aromatic) price	Normal distribution	21.12
Hydrogen price	Normal distribution	19.33
LPG price	Normal distribution	10.32
Fuel Oil price	Normal distribution	18.75
Water price	Normal distribution	9.08
Financial evaluation	Uniform random distribution	25.00
Environmental impact	Uniform random distribution	20.00

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