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Synthesis of Cresols and Xylenols from Benzene and Methanol

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- EXECUTIVE SUMMARY -

The objective of the work is to compare two (2) processes for manufacturing cresols and xylenols: a) -a conventional catalytic process, and b) -a photo-thermal catalytic process, in order to determine the relative process economics. The products are used primarily as chemical intermediates for manufacture of antioxidants, pesticides, polymerization inhibitors, resins, and other products. The market is approximately 500 million pounds per year.

This report is the <u>second</u> of two reports, presenting results of a process evaluation for manufacturing the products by a <u>photo-thermal catalytic process.</u>.

At the outset, as experimental data are not yet available to provide a definitive design basis, a series of assumptions were made in order to proceed with the evaluation. As regards capacity, an arbitrary <u>base case</u> plant size (fresh feed) of approximately 7.06 million kg/y (15.6 million lbm/y) was chosen, and then the economics scaled to break-even size. Calculations indicated the following comparative numbers:

<u>BASE CASE:</u>

1) Plant Size, fresh feed = 7.056 E6 kg/y; products = 5.192 E6 kg/y

2)	Plant Capital Cost	\$ 2.111 E6
3)	Plant Operating Cost (POC)	\$ 3.361 E6
4)	Plant Income (PI)	\$ 7.267 E6
5)	PI/POC	2.162
6)	Minimum Q_{solar}	168 kW

<u>BREAK-EVEN CASE:</u>

1) Plant Size, fresh feed = 1.652 E6 kg/y; products = 1.215 E6 kg/y

2)	Plant Capital Cost	\$ 0.8833 E6
3)	Plant Operating Cost and Income	\$ 1.701 E6
4)	Minimum Q_{solar}	40 kW

The above capital costs are for process equipment only, and <u>do not</u> include equipment to deliver solar energy to the top of the reactor

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The evaluation indicates that for the photo-catalytic process, the break-even capacity is only about 24% of the base case, and about the same percentage of the conventional catalytic process (Report #1). Assuming the total capital cost would double, which is unlikely, when the solar energy equipment is included, the overall conclusion in favor of the photo-catalytic process would not change.

TABLE OF CONTENTS

(9-30-89)

- INTRODUCTION -

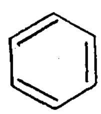
This report is the <u>second</u> of two report concerning the manufacture of cresols and xylenols by, 1) -a conventional catalytic process, and 2) -a solar-thermal photo-catalytic process. The two reports when complete will provide a preliminary basis for comparison of the relative process economics.

The purpose of this report is to present the work accomplished on sizing and costing a <u>solar photo-thermal catalytic process</u> to produce the products from benzene and methanol. No process configuration, sizing, and costing were available; therefore, a series of assumptions were made in order to carry out the necessary calculations to obtain process details and the economics. The method for comparison of the two processes was to determine the "break-even" capacity for each process.

At the outset the reader should become familiar with the structures of the product compounds, in order to visualize the synthesis chemistry. In the photo-catalytic reaction, conducted with a large excess methanol, the benzene provides the ring structure and the methanol provides the methyl group (by alkylation) and the hydroxyl group (by hydroxylation).

The reactants:

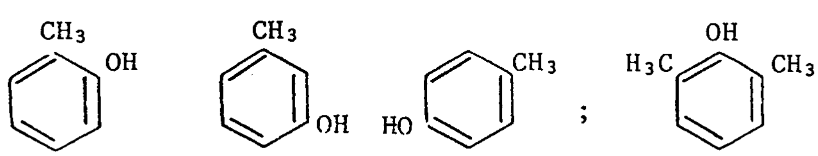
benzene
C_6H_6
M=78.113



; methanol H_3C-OH
M=32.042

and the products:

cresols
C_7H_8O
M=108.14



ortho- meta - para - 2,6-xylenol

$C_8H_{10}O$
M=122.17

Cresol and xylenol isomers are used primarily as chemical intermediates. Principal applications include use for: anti- oxidants, pesticides, polymerization inhibitors, resins, and other miscellaneous uses. The annual consumption of the products [2] was presented in the first report, as well as the U.S. price history; current reactant and product prices are presented in Appendix B.

1.00 PROCESS DESCRIPTION AND DESIGN BASIS

At the outset, as experimental data are not yet available to provide a definitive design basis, the following assumptions were made in order to proceed with an economic evaluation of the process.

1. The overall reaction stoichiometry for the process is,

$$C_6H_6 + 5\ CH_3OH \longrightarrow 0.50\ o\text{-}C_7H_8O + 0.50\ m,p\text{-}C_7H_8O + 0.50\ C_8H_{10}O + 3.50\ H_2O + 3.00\ H_2$$

For this endothermic reaction the $\Delta Hr^0(298K) = 595,100$ kJ/kgmole benzene.

2. The Reaction Section of the plant will operate only during "sun hours"= 2500 h/y; while the Separation Section of the plant will operate 24 h/d = 8400 h/y (downtime = 360 h/y). The solar scale-factor becomes 8400/2500 = 3.36

3. The fresh feed and production rates are:

Fresh Feed	7.056 million kg/y = 15.56 million lbm/y
o-Cresols	1.601 million kg/y = 3.530 million lb/y
m,p-Cresols	1.601 million kg/y = 3.530 million lb/y
Xylenols	1.809 million kg/y = 3.988 million lb/y
Hydrogen	0.1791 million kg/y = 0.3948 million lb/y

4. Solar energy input, in an amount necessary to supply the reaction energy requirement, will be sufficient to provide the necessary VIS-UV energy to activate the catalyst.

5. The plant is a process unit within an existing chemical plant where utilities and other services are available.

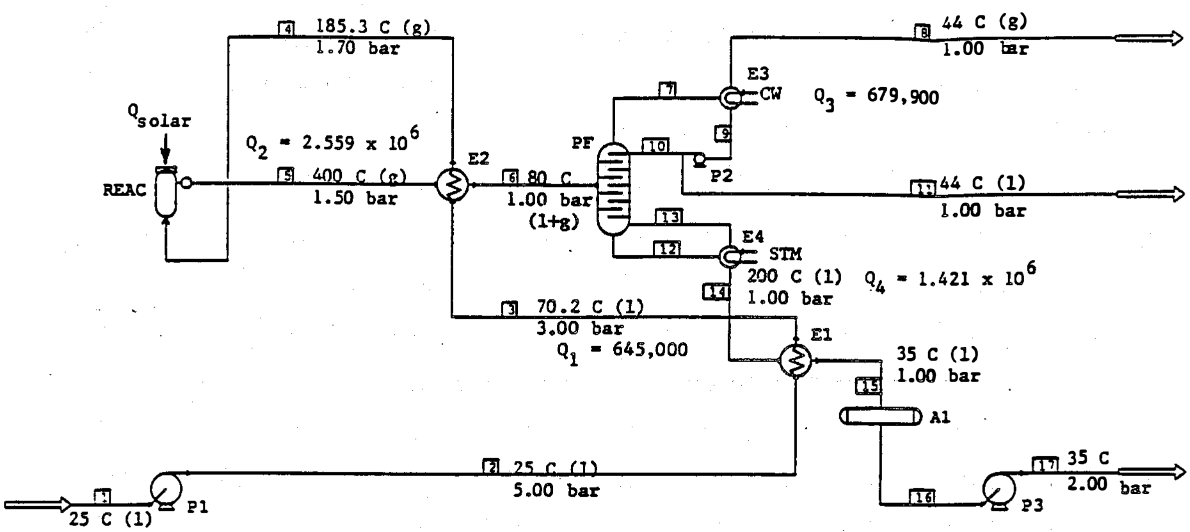
The reader is referred to Figure 1 (p4) Process Flow - Reaction Section, and Figure 2 (p6) Process Flow - Separation Section. A mass balance at key points through the process, as well as process conditions, are shown on the diagrams. Because the Reaction Section would operate on a reduced number of hours/day, whereas the Separation Section would operate 24 h/d, a "solar scale factor, Sf = 3.36" has been included, which means that on a yearly-average the Reaction Section would operate 24/3.36 = 7.14 h/d.

The process flow for the Reaction Section (refer to Figure 1) proceeds as follows. Fresh feed as liquid (benzene and methanol) enters as stream 1, is pumped as stream 2 through heat exchanger E1 to recover heat from the cresol-xylenol bottoms stream (14) from the primary fractionator (PF). The feed stream, 3, flows through exchanger E2 to pick up additional heat and vaporize before entering the reactor (REAC). The heat transferred in E2 is provided by cooling the reactor effluent stream 5. In the reactor the feed is converted to products by the overall stoichiometry shown above. In heat exchanger E2 the reactor effluent is partially condensed and flows as stream 6 to the primary fractionator (PF). The primary function of PF is to remove the hydrogen as stream 8, the water as stream 11, and the cresols and xylenols as the bottoms stream 14. The overhead condenser loop is the stream sequence 7, 8, 9, 10, and the reboiler loop is streams 12,13,14. After giving up heat in E1, the excess flow of stream 15 is partially stored in accumulator A1, while the flow to the Separation Section is stream 17.

The process flow for the Separation Section, Figure 2 (p5), proceeds as follows. The accumulated material in A1 is pumped as stream 17 where it is divided into streams 18, 20 and 21. Stream 18 flows through heat exchanger E5 to recover heat from the cresol overhead stream (27) from the o-cresol-xylenol separation column (OCX) and exits as stream 22. Stream 20 enters heat exchanger E6 where it recovers heat from the xylenol bottoms stream (34) from the cresol-xylenol separation column (CX) and exits as stream 23. Stream 21 flows through heat exchanger E7 to recover heat from the cresol overhead stream (31) from CX and exits as stream 24. Streams 22, 23 and 24 recombine and enter the o-cresol-xylenol separation column (OCX). The main function of OCX is to separate o-cresol as overhead stream 27 and m,p-cresol and xylenol as bottoms stream 29. Stream 27 is cooled in E5 and enters the o-cresol storage tank as stream 28. The OCX bottoms stream is pumped as stream 30 where it enters the cresol-xylenol separation column (CX). The primary function of CX is to remove m,p-cresols as overhead stream 31 and xylenol as bottoms stream 34. Stream 31 is cooled in E7 and exits to the xylenol storage tank as stream 32. Stream 34 is cooled in E6 and enters the m,p-cresol storage tank as stream 35.

The major pieces of equipment are:

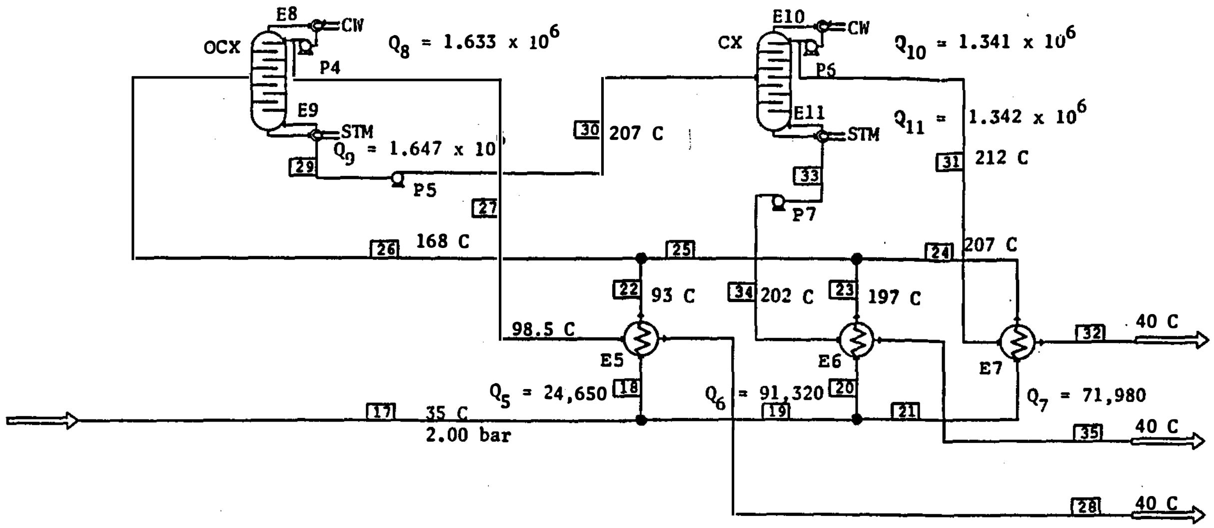
1-reactor, 3-fractionators, 4-accumulators, 11-heat exchangers, 7-pumps, and 5-storage tanks.



Solar Factor, S_f = 3.36 — streams and flow rates, kg/h

Component	M.W.	1	5	14,15	8	11	17
a) BENZENE	78.113	925.17	0.0000	0.0000	0.0000	0.0000	0.0000
b) METHANOL	32.024	1897.5	0.0000	0.0000	0.0000	0.0000	0.0000
c) o-CRESOL	108.14	0.0000	640.41	640.41	0.0000	0.0000	190.59
d) m-CRESOL	108.14	0.0000	320.20	320.20	0.0000	0.0000	95.293
e) p-CRESOL	108.14	0.0000	320.20	320.20	0.0000	0.0000	95.293
f) MIXED XYLENOLS	122.17	0.0000	723.49	723.49	0.0000	0.0000	215.31
g) WATER	18.02	0.0000	747.04	0.0000	3.2300	747.04	0.0000
h) HYDROGEN	2.016	0.0000	71.633	0.0000	32.302	0.0000	0.0000
		2822.7	2823.0	2004.3	123.326	747.04	596.49

Figure 1. PROCESS FLOW - REACTION SECTION
(Note: Q-Values are kJ/h)



streams and flowrates, kg/h

Component	M.W.	17,26	27,28	29,30	31,32	34,35
g) WATER	18.02	1.1118	1.1118	0.0000	0.0000	0.0000
c) o-CRESOL	108.14	190.33	188.42	1.9033	1.9033	0.0000
d) m-CRESOL	108.14	95.300	0.0953	95.208	94.254	0.9521
e) p-CRESOL	108.14	95.300	0.1062	95.197	94.518	0.6768
f) MIXED XYLENOLS	122.17	215.32	0.0000	215.32	0.4306	214.89
		597.4	189.7	407.6	191.1	216.5

Figure 2. PROCESS FLOW - SEPARATION SECTION
(Note: Q-Values are kJ/h)

2.00 CHEMICAL REACTION/REACTOR SECTION

The Reaction Section is the most important part of the plant as it carries out the conversion of feedstock to synthesized products. In this part of the report the details of the Reaction Section are presented.

The reader is referred to the flow diagram, Figure 1, where the stream numbers, temperatures, pressures, and heat exchanger Q-values are shown on the diagram. Table 1 presents the stream masses, compositions, conditions, and enthalpies for key streams in the Reaction Section. It will be noted that the solar energy input can be calculated by,

$$Q_{solar} = m\Delta H = m_5H_5 - m_4H_4 = -9.579\ E6 - (-10.183\ E6)$$

$$= 0.605\ E6\ kJ/h\ (\text{endothermic}) = 168\ kW$$

which assumes that within this total "thermodynamic" amount of energy there is sufficient VIS-UV to photo-activate the catalyst. At present it is our expectation that the final amount will not be more than 2 or 3 times the above calculated value. If the value turns out to be more than the thermodynamic value, then the excess would be used to generate steam, and a credit taken on the utility bill. A measured value of the energy requirement is yet to be determined by Wemtworth's Research Group.

Sizing and costing calculations were made for the shallow (h/D = 1/4) fluidized bed reactor, and are summarized in Table 2. The reactor size is approximately: 45"i.d. x 10' s to s, with a 2' dia. quartz window in the top; the reactor would be lined with high temperature refractory cement, which is typical of commercial fluid-bed catalytic reactors.

Table 1. Stream Masses, Compositions, Conditions & Enthalpies

Datum state: enthalpies and entropies = 0, for the chemical elements in their naturally occuring physical state at 298.16 K. Liquid phase mixing enthalpies are assumed small cf. formation enthalpies.

Components: benzene (a), methanol (b), o-cresol (c), m-cresol (d), p-cresol (e), mixed xylenols (f), water (g), and hydrogen (h).

Reaction Section (S_f = 3.36)

Stream	kg/h kgmols/h		composition x	composition y	conditions T,P	enthalpies kJ/kgmol	enthalpies kJ/h
2 (L)	2822.1 71.050	a b	0.1667 0.8333		25 C = 298 K 5.00 bars	H_2 = - 188,407	m_2H_2 = - 13.386E6
3 (L)	(")		(")		70.2 C = 343.2 K 3.00 bars	H_3 = - 179,336	m_3H_3 = - 12.74E6
4 (G)	(")	a b		0.1667 0.8333	185.3 C = 458.3 K 1.70 bars	H_4 = - 143,320	m_4H_4 = - 10.183E6
5 (G)	2823.4 94.769	c d e f g h		0.0625 0.0313 0.0313 0.0625 0.4375 0.3750	400 C = 673 K 1.50 bars	H_5 = - 101,082	m_5H_5 = - 9.5796E6

Table 1. (continued)

Stream	kg/h kgmols/h		composition x	composition y	conditions T,P	enthalpies kJ/kgmol	enthalpies kJ/h
6 (L+G)	(")	c	0.1139	0.0018	80 C = 353 K	H_6 = - 128,086	m_6H_6 = - 12.14E6
		d	0.0595	0.0005	1.00 bar		
		e	0.0633	0.0005			
		f	0.1216	0.009			
		g	0.5785	0.2767			
		h	0.0727	0.7197			
8 (G)	71.60	g		0.0909	44 C = 317 K	H_8 = - 21,399	m_8H_8 = - 0.7604E6
	35.532	h		0.9091	1.00 bar		
11 (L)	746.81	g	1.0000		44 C = 317 K	H_{11} = - 281,281	$m_{11}H_{11}$= -11.66E6
	41.455				1.00 bar		
14 (L)	2004.9	c	0.3333		470 C = 743 K	H_{14} = - 146,411	$m_{14}H_{14}$= - 2.6002E6
	17.772	d	0.1667		1.00 bar		
		e	0.1667				
		f	0.3333				
15 (L)	596.69		(")		35 C = 308 K	H_{15} = - 182,691	$m_{15}H_{15}$= - 3.247E6
	5.289				1.00 bar		
17 (L)	(")		(")		35 C = 308 K	H_{17} = -182,691	$m_{17}H_{17}$= - 09663E6
					2.00 bars		

1 bar = 14.504 psia
1 BTU = 1.055 kJ

Table 2. REACTOR SPECIFICATIONS

Item	Description
1) Type	Fliuidized Bed w/top entry solar energy; w/cyclone separator on discharge
2) Catalyst	124 kg; 3 w% V_2O_5 on SiO_2 support 60-80 micron particle size; 300 m^2 surf. area catalyst bed density = 0.431 g/cm^3 = 26.9 lbm/ft^3
3) Bed dimensions	1.134 m dia x 0.284 m ht. volume = 0.2863 m^3 = 10.11 ft^3 c.s. area = 1.010 m^2 = 10.87 ft^2
4) Vessel dimens.	45" i.d. x 12' s to s; 2' dia top quartz window, catalyst bed support grid; conical bottom; two-stage cyclone separator

. Operating Conditions .

	entrance	exit
5) Flow rate	71.063 kgmols/h 2822.7 kg/h	94.763 =
6) T,P	185 C, 1.70 bar	400 C, 1.50 bar
7) Gas density	1.774 kg/m^3	0.7989 kg/m^3
8) Space velocity	22.76 kg/h kg cat.	
9) Mass velocity	2795 kg/h m^2	
10) Min. fluidization mass velocity	1982 kg/h m^2	
11) Q solar*	0.604 kJ/h = 168 kW	

12) Material of construction:	carbon steel shell, catalyst grid support, hi-temp refractory cement lining, top quartz window; carbon steel (w/liner) cyclone
13) Estimated Cost:	$ 31,210

* Based on thermodynamic requirement

3.00 EQUIPMENT SIZING AND COST

Specifications and costs for the individual pieces of equipment are presented in Tables 4-7 incl. Costs were estimated using the functions and charts given by Guthrie [5] based on 1974 data, which were escalated to 1989. The cost escalation index (see Appendix C) was calculated by, I(1974) = 202.5, I(1989) = 391.0, giving Ic = 391.0/202.5 = 1.931.

The costs by equipment catagory are summarized in Table 3, as follows.

Table 3. SUMMARY OF EQUIPMENT COSTS
(fresh feed = 7.056 million kg/y = 15.56 million lbm/y)

catagory	number	Cost ($)
1) Reactor w/2-stage Cyclone	(1)	31,210
2) Heat exchangers	(11)	126,435
3) Distillation columns	(3)	118,230
4) Accumulators (A1, 5d storage)	(4)	61,170
5) Pumps with spares	(7)	18,100
6) Storage tanks	(4)	191,100
		(546,245)
7) Process Instruments & Controls (15%)		81,937
8) Computer (data logging & control)	(1)	110,000
9) Catalyst, initial charge	(1)	1,000
Total Equipment		$739,200

Table 4 - HEAT EXCHANGER SUMMARY

	Duty kJ/h	Fluids TS/SS	T_{in} (C)	T_{out}	ΔT_{Lm} U Area	MC	Estimated Cost
E1 Feed Heat Exchanger	0.645E6	Feed PF Btm	25 200	70.2 35	46.7 K 1020 13.54 m^2 = 145.7 ft^2	304 SS CS	$ 7445
E2 Reactor Economizer	2.559E6	Feed Reac. Pro.	70.2 400	185.3 80	66.83 2860 13.48 = 145	304 SS CS	$ 12,342
E3 PF Col. Condenser	0.6799E6	CW PF Ovhd	32 83	49 83	41.93 2247 7.22 = 77.7	304 SS CS	$ 7611
E4 PF Col. Reboiler	1.421E6	Steam PF Btm	242 171	242 171	71.00 2860 7.00 = 75.3	304 SS CS	$ 7451
E5 OCX Heat Exchanger	0.02465E6	PF Btm o-Cresol	35 98.5	93 40	5.25 1022 4.59 = 49.43	304 SS CS	$ 3519
E6 Xyl. Heat Exchanger	0.09132E6	PF Btm Cresol	35 202	197 40	5.00 1022 17.87 = 192.3	304 SS CS	$ 9549

Table 4 - HEAT EXCHANGER SUMMARY (continued)

	Duty kJ/h	Fluids TS/SS	T_{in} (C)	T_{out}	ΔT_{Lm} U Area	MC	Estimated Cost
E7 CX Heat Exchanger	0.07198E6	PF Btm Xylenol	35 212	207 40	5.00 1022 14.09 = 151.6	304 SS CS	$ 7703
E8 OCX Col. Condenser	1.633E6	CW OCX Ovhd	32 98.5	49 98.5	57.58 1737 16.33 = 175.7	304 SS CS	$ 14,884
E9 OCX Col. Reboiler	1.647E6	Steam OCX Btm	242 207	242 207	35.00 1430 32.91 = 354.1	304 SS CS	$ 25,262
E10 CX Col. Condenser	1.341E6	CW CX Ovhd	32 203	49 203	162.4 1737 4.75 = 51.15	304 SS CS	$ 6262
E11 CX Col. Reboiler	1.342E6	Steam CX Btm	242 212	242 212	30.00 1430 31.28 = 336.6	304 SS CS	$ 24,407

Total ($) 0.1264E6

Table 5a. PF Distillation Column

Feed stream 6; overhead stream 7; bottoms stream 12

Parameter		Top of column	Bottom of column
Z, comp. factor		1	1
Temperature	C	83	171
Pressure	atm	1	1
Liq. density	kg/m^3	969.8	936.124
Gas density	kg/m^3	0.3596	3.0267
Gas av. mol. wt.		10.622	111.73
Liq. surface tension	dyn/cm	19.66	25.04
Feed flow	kg/h	2823	
Vapor fraction in feed		0.726	
Reflux ratio		0.2108	
Dist. flow	kg/h	815.61	
Gas flow	kg/h	987.56	1062
Liq. flow	kg/h	171.95	3069
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.0034	0.1643
Tray spacing	in.	18	18
K	ft/s	0.2738	0.2205
Vmax	m/s	4.1	1.17
Gmax	kg/hm^2	5311	12777
"Active" area	m^2	0.17	0.08
Calc. column dia.		0.5 m = 1.64 ft	

Condenser type		partial
Feed flow	kg/h	2823
Feed temperature	C	80
LK/HK		water/o-cresol
Recovery of LK in overhead	%	99.5
Recovery of HK in overhead	%	0.1
Actual stages		40
Operating reflux ratio		0.2108
Feed stage		23 top down
Condenser duty	kJ/h	6.799E5
Reboiler duty	kJ/h	1.421E6
Overhead temperature	C	83
Bottom temperature	C	171
Distillate flow	kg/h	815.61
Bottom flow	kg/h	2008
Design pressure	psig	200

Column dimensions [d x h (s to s)]	2' id x 68.5'
MC	CS/304 SS
Estimated Cost	$26,640

Table 5b. OCX Distillation Column

Feed stream 26; overhead stream 27; bottoms stream 29

Parameter		Top of column	Bottom of column
Z, comp. factor		0.9747	1
Temperature	C	98.5	207
Pressure	atm	1	1
Liq. density	kg/m^3	965.488	917.56
Gas density	kg/m^3	2.802	2.8848
Gas av. mol. wt.		105.061	115.124
Liq. surface tension	dyn/cm	19.66	25.04
Feed flow	kg/h	597.367	
Vapor fraction in feed		0.00	
Reflux ratio		12.68	
Dist. flow	kg/h	189.735	
Gas flow	kg/h	2073.2	2073.2
Liq. flow	kg/h	1883.4	2480.8
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.0489	0.0671
Tray spacing	in.	18	18
K	ft/s	0.2573	0.2510
Vmax	m/s	1.38	1.35
Gmax	kg/hm^2	13883	14058
"Active" area	m^2	0.15	0.15
Calc. column dia.		0.44 m = 1.44 ft	
Condenser type			total
Feed flow		kg/h	597.4
Feed temperature		C	168
LK/HK			o-cresol/m-cresol
Recovery of LK in overhead		%	99
Recovery of HK in overhead		%	0.1
Actual stages			82
Operating reflux ratio			12.684
Feed stage			50 top down
Condenser duty		kJ/h	1.633E6
Reboiler duty		kJ/h	1.647E6
Overhead temperature		C	99
Bottom temperature		C	207
Distillate flow		kg/h	189.7
Bottom flow		kg/h	407.6
Design pressure		psig	200
Column dimensions [d x h (s to s)]			2' id x 131.5'
MC			CS/304 SS
Estimated Cost			$47,890

Table 5c. CX Distillation Column

Feed stream 30; overhead stream 31; bottoms stream 33

Parameter		Top of column	Bottom of column
Z, comp. factor		0.9734	1
Temperature	C	203	212
Pressure	atm	1	1
Liq. density	kg/m^3	861.148	973.194
Gas density	kg/m^3	2.8099	3.0584
Gas av. mol. wt.		108.168	122.051
Liq. surface tension	dyn/cm	23.88	25.26
Feed flow	kg/h	407.627	
Vapor fraction in feed		0.00	
Reflux ratio		14.467	
Dist. flow	kg/h	191.106	
Gas flow	kg/h	2974.9	2974.9
Liq. flow	kg/h	2783.8	3191.5
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.0535	0.0601
Tray spacing	in.	18	18
K	ft/s	0.2557	0.2534
Vmax	m/s	1.34	1.37
Gmax	kg/hm^2	13555	15084
"Active" area	m^2	0.22	0.20
Calc. column dia.		0.53 m = 1.74 ft	

Condenser type		total
Feed flow	kg/h	407.6
Feed temperature	C	207
LK/HK		m-cresol/xylenol
Recovery of LK in overhead	%	99
Recovery of HK in overhead	%	0.2
Actual stages		70
Operating reflux ratio		14.567
Feed stage		42 top down
Condenser duty	kJ/h	1.341E6
Reboiler duty	kJ/h	1.342E6
Overhead temperature	C	203
Bottom temperature	C	212
Distillate flow	kg/h	191.1
Bottom flow	kg/h	216.5
Design pressure	psig	200

Column dimensions [d x h (s to s)]	2' id x 113.5'
MC	CS/304 SS
Estimated Cost	$43,700

Table 6. PUMP SUMMARY

(Centrifugal, stainless; costs for pump + spare + motor)

Pump	Inlet stream	Capacity (gpm)	ΔP(psi)	BHP	Cost($)
P1	1	16	500	5.62	5973
P2	9	3	135	0.29	1928
P3	16	3	135	0.24	1892
P4	from E8	2	135	0.86	2109
P5	29	9	135	0.16	1904
P6	from E10	13	135	1.25	2402
P7	33	1	135	0.08	1908

Total $18,100

Table 7. STOARAGE TANK SUMMARY

(Based on approximate 10-day storage time, except 5 days for methanol)

Tank	Substance	Density (kg/liter)	Capacity (U.S. Gallons)	MC	Estimated Cost(1988)
T1	Benzene	0.879	67,000	CS	$71,900
T2	Methanol	0.792	75,000	CS	80,500
T3	o-Cresol	1.048	12,000	CS	12,900
T4	m,p-Cresol	1.035	12,000	CS	12,900
T5	Xylenol	1.1695	12,000	CS	12,900

Total $191,100

4.00 ESTIMATED CAPITAL AND OPERATING COSTS

The methods used to calculate the process economics follow standard chemical engineering procedures as presented by Guthrie [5], Peters and Timmerhaus [6], and Perry's Handbook [7].

Table 8. Estimated Capital Cost
(fresh feed = 7.056 million kg/y = 15.56 million lbm/y)

Item	factor	$/1000
A. Equipment (Table 3)		739.2
B. Interconnecting piping, flanges, fittings, valves	(15% A)	110.9
C. Assembly and Installation of Equipment		
purchasing, materials, labor and supervision	(40% A)	295.7
foundations and structures	(30% A)	221.8
running pipe, steam tracing, insulation, painting	(20% A)	147.8
electrical	(10% A)	73.9
		(1589.3)
D. Design and Engineering	(8% A+B+C)	127.1
E. BASE SYSTEM COST (BSC)		1716.4
F. Contractors fee	(8% BSC)	137.3
G. Contingency	(15% BSC)	257.5
H. TOTAL INSTALLED PLANT COST		$ 2.111 E6

It has been shown by a number of authors [5,6,7] that plant capital cost can be correlated by a 6-tenths-power relationship. For this plant [$F = 7.056 \times 10^6$ kg/y, Ic (1989) = 1.931] the equation becomes,

$$C(\$) = Co\ Ic\ F^{0.60} = (85.029)\ Ic\ F^{0.60}$$

which can be used as the capital cost scaling-equation for different size plants. For example, for a plant of F = 14 E6 kg/y the estimated cost is $ 3.184 E6 .

The estimated plant operating cost is presented in Table 9. It is assumed that the plant is a process unit within an existing chemical plant where necessary utilities and other services are available.

Table 9. Plant Operating Cost
(2500 sun hours; 8400 operating h/y)

Item	$/y
1) Raw Materials (benzene, methanol, supplies, make-up catalyst)	1.648 E6
2) Operating labor & supervision (3-operators, 1-technicial, 1/2 foreman, per shift)	0.5292
3) Utilities (nat'l gas, steam, cooling water, electric power)	0.09125
4) Maintenance & Repair (7% of capital cost/y)	0.1478
5) Plant overhead (75% operating labor)	0.3969
6) Plant G/A (25% operating labor)	0.1323
7) Depreciation (15 y life, loan payment)	0.1407
8) Interest on borrow capital (10%/y, 15 y, on declining balance)	0.2111
9) Taxes and Insurance (3% of capital cost/y)	0.0633
10) TOTAL OPERATING COST	$ 3.361 E6
11) Unit COST of PRODUCTS SOLD (3.361/11.443)	$ 0.2937 /lbm $ 0.6475 /kg

The profitability analysis and break-even capacity now can be calculated !

5.00 PROFITABILITY ANALYSIS

Now it is necessary to determine whether or not the base case plant size would be a profitable venture. First, the plant income from sale of products can be calculated, as shown in Table 10.

Table 10. Plant Income from Products

product	lbm/y	$/lbm	$/y
1) hydrogen	0.3948 E6	0.0307	12120
2) o-Cresol	3.530 E6	0.580	2.047 E6
3) m,p-cresols	3.350 E6	0.820	2.895 E6
4) mixed Xylenols	3.988 E6	0.580	2.313 E6
5) Totals	11.443 E6		7.267 E6
6) Average unit income (7.267/11.443)			$ 0.6351/lb $ 1.400/kg

Comparing the average $/lbm income with the cost/lbm (Table 9) it is obvious that the base case is beyond break-even, and the capacity will have to be reduced to find the break-even point. The operating cost items in Table 9 can be written in equation form and programed as a function of plant capacity; some items are directly proportional and some less than proportional to size (e.g. capital cost), while others are constant. Table 11 presents a print-out for determination of the <u>first-year break- even</u> point, giving the following values:

1) Fresh Feed	(7.056 E6)(0.2341) =	1.652 E6 kg/y
2) Products	(5.192 E6)(0.2341) =	1.215 E6 kg/y
3) Capital Cost		$ 0.8833 E6
4) Op-Cost & Income		$ 1.701 E6/y

The qualifier "first-year" is used because the interest payment declines each year as the principal is reduced.

Finally, the work described herein permits the following evaluative conclusions to be drawn for the process:

1. -a plant producing greater than 2.679 E6 lbm/y = 1.215 E6 kg/y of products would be a profitable venture.

2. -the configuration of the process indicates the equipment complexity, which directly affects the capital investment required.

3. -the major item of operating cost is raw materials - 49% of total.

4. -the report provides a basis for comparison with the Conventional Catalytic Process described in the first report. Because of lower raw

Table 11. Calculation of First-Year Break-Even Capacity

SYMBOLS & NOMENCLATURE

C	plant cost ($)
F, Fo	fresh feed, base case fresh feed (kg/y)
Inc	annual income ($/y)
Rm	raw material cost ($/y)
Sf	plant capacity scale factor, F/Fo
Top	plant operating cost ($/y)

TABLE 1 - Base Case Size

Fo(kg/y)
7056000

TABLE 2 - Profitability Analysis as f(plant capacity)

J	Sf	C($)	Rm($)	Top($)	Inc($)	Inc/Top
1	0.1842	765095	303628	1582891	1338875	0.8458
2	0.1984	799883	326984	1616818	1441865	0.8918
3	0.2126	833689	350340	1650484	1544855	0.9360
4	0.2268	866606	373696	1683912	1647846	0.9786
5	0.2341	883300	385771	1701108	1701092	1.0000
6	0.2551	930064	420408	1750134	1853827	1.0592
7	0.2834	990758	467120	1815620	2059807	1.1345
8	0.5669	1501708	934240	2444875	4119614	1.6850
9	0.8503	1915315	1401361	3048169	6179422	2.0273
10	1.0000	2110983	1648000	3360649	7267000	2.1624

Out of Data
END OF CALCULATION (9-26-89)

material cost and higher income, the break-even size was significantly lower for the Solar-Catalytic Process.

5. -the capital cost estimate is for the chemical process equipment, and does not include the cost of equipment to deliver the solar energy to the top of the reactor. Assuming the total capital cost would double, which is unlikely, when the solar energy equipment is included, the conclusion in favor of the photo-catalytic process would not change.

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[5] Schnell Publishing Co., Inc., Chemical Marketing Reporter, 19 June 1989 issue.

A1 - Benzene, C_6H_6

1) Molecular Weight, M — 78.113

2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 562.16, 48.34, 258.94, 0.274

3) Acentric factor; dipole moment — $\omega = 0.209$, $\mu = 0.0$ D

4) T_{tp}(K), T_b (K) — 278.66, 353.3

5) At 293.16K, ρ_1 (g/cm^3) — 0.879

6) At 298.16K

	Cp(1)	Cp°	S°	ΔH^v	$\Delta H_f°$	$\Delta G_f°$
a)	32.11	19.52	64.34	7.352	19.82	30.99
		(cals/gmol, K)			(kcals/gmol)	
b)	134.35	81.71	269.33	30,761	82,926	129,662
		(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_1 = 12.26\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Liquid density, $\ln \rho_1 = -0.024098 + 1.344347\ [1 + (1 - T/0.56216E3)^{0.27357}]$ (kgmol/m^3)

3) Vapor pressure: $\ln P\ (\text{torr}) = 16.1753 - 2948.78/(T - 44.563)$

$\ln P\ (\text{atm}) = 10.0114 - 3291.87/T - 84994.9/T^2$

4) Mole $Cp°/R = -2.69988 + 4.83994E\text{-}2\ T - 2.06081E\text{-}5\ T^2$

5) Mole Cp(1) = 32.3793 + 0.342T, (kJ/kgmol, K)

6) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

7) Surface tension, $\sigma = 0.07195\ (1 - T_r)^{1.2389}$, (N/m)

8) Viscosity, vs: $\log \text{vs}\ (\text{cp}) = 545.64\ (1/T - 1/265.34)$

A2 - Methanol, CH_3OH

1) Molecular Weight, M — 32.042
2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 512.58, 79.9, 117.8, 0.222
3) Acentric factor; dipole moment — $\omega = 0.5656$, $\mu = 1.70$ D
4) T_{tp}(K), T_b (K) — 175.7, 337.8
5) At 293.16 K, ρ_1 (g/cm^3) — 0.792
6) At 298.16 K

	$Cp(1)$	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	46.52	10.49	57.29	8.426	-48.08	-38.84
	(cals/gmol, K)			(kcal/gmol)		
b)	194.7	43.9	239.8	35,271	-201,263	-162,584
	(kJ/kgmol, K)			(kJ/kgmol)		

Equations

1) Liquid volume, $V_1 = 5.4628\ (5.7 + 3T_r)$, ($cm^3$/gmol)
2) Liquid density, $\ln \rho_1 = 0.18706 + 1.62055\ [1 + (1 - T/0.51263E3)^{0.17272}]$, ($kgmol/m^3$)
3) Vapor pressure: $\ln P\ (torr) = 18.5097 - 3593.39/(T - 35.225)$

   $\ln P\ (atm) = 11.9921 - 3679.33/T - 126059/T^2$
4) Mole $Cp^o/R = 1.85019 + 0.0124255\ T - 3.49129E{-6}\ T^2$
5) Mole $Cp(1) = -39.9665 + 0.787208\ T$, (kJ/kgmol, K)
6) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$
7) Surface tension, $\sigma = 0.04327\ (1 - T_r)^{0.7676}$, (N/m)
8) Viscosity, vs: $\log vs\ (cp) = 555.3\ (1/T - 1/260.64)$

A3 - o - Cresol, C_7H_8O

1) Molecular Weight, M — 108.14

2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 697.55, 49.4, 282.0, 0.249

3) Acentric factor; dipole moment — $\omega = 0.434$, $\mu = 1.60$ D

4) T_{tp}(K), T_b (K) — 304.0, 464.2

5) At 293.16 K, ρ_l (g/cm^3) — 1.048

6) At 298.16 K

	Cp(l)	Cp°	S°	ΔH^v	$\Delta H_f°$	$\Delta G_f°$
a)	55.29	31.15	85.47	10.80	-30.74	-8.86
		(cals/gmol, K)			(kcal/gmol)	
b)	231.4	130.4	357.8	45,209	-128,678	-37,088
		(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_l = 14.9288\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Liquid density, $\ln \rho_l = 0.58912 + 1.18685\ [1 + (1 - T/0.69755E3)^{0.3099}]$, ($kgmol/m^3$)

3) Vapor pressure: $\ln P\ (torr) = 16.2829 - 3552.74/(T - 95.975)$

$\ln P\ (atm) = 11.1411 - 4406.52/T - 351528/T^2$

4) Mole $Cp°/R = 1.40132 + 0.0552621\ T - 2.28792E\text{-}5\ T^2$

5) Mole $Cp(l) = 559.336 - 1.86259\ T + 0.2258292E\text{-}2\ T^2$, (kJ/kgmol, K)

6) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

7) Viscosity, vs: $\log vs\ (cp) = 1785.6\ (1/T - 1/370.75)$

A4 - Water, H_2O

1) Molecular Weight, M — 18.02

2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 647.35, 218.29, 63.494, 0.230

3) Acentric factor; dipole moment — $\omega = 0.348$, $\mu = 1.80$ D

4) T_{tp}(K), T_b (K) — 273.16, 373.15

5) At 277.16 K, ρ_1 (g/cm^3) — 1.00

6) At 298.16

	Cp (1)	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	18.02	8.03	45.11	9.717	-57.8	-54.64
	(cals/gmol, K)			(kcal/gmol)		
b)	75.4	33.6	188.8	40,675	-241,951	-228,723
	(kJ/kgmol, K)			(kJ/kgmol)		

<u>Equations</u>

1) Liquid volume, $V_1 = 2.552\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Liquid density, $\ln \rho_1 = 1.52903 + 1.33888\ [1 + (1 - T/0.64729E3)^{0.23072}]$, ($kgmol/m^3$)

3) Vapor pressure: $\ln P\ (torr) = 18.3036 - 3816.44/(t - 46.13)$

$\ln P\ (atm) = 11.6572 - 3761.58/T - 218339/T^2$

4) Mole $Cp^o/R = 2.37293 + 0.0160161\ T - 7.40155E{-6}\ T^2$

5) Mole $Cp(1) = 32.4953 + 0.124601\ T$, (kJ/kgmol, K)

6) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

7) Surface tension, $\sigma = 0.1386\ (1 - T_r)^{1.6866}$, (N/m)

8) Viscosity, vs: $\log vs\ (cp) = 656.25\ (1/T - 1/238.16)$

A5 - m - Cresol, C_7H_8O

1) Molecular Weight, M — 108.14

2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 705.8, 45.0, 310.0, 0.248

3) Acentric factor; dipole moment — ω = 0.464, μ = 1.80 D

4) T_{tp}(K), T_b (K) — 284.1, 475.4

5) At 293.16 K, ρ_l (g/cm^3) — 1.034

6) At 298.16 K

	$Cp(l)$	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	55.29	29.27	85.27	11.33	-31.63	-9.69
		(cals/gmol, K)			(kcal/gmol)	
b)	231.4	122.5	356.9	47,427	-132,403	-40,562
		(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_l = 15.0581\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Vapor pressure: $\ln P\ (\text{torr}) = 18.3036 - 3816.44/(T - 46.13)$

$\ln P\ (\text{atm}) = 7.66037 - 1479.07/T - 1030280/T^2$

3) Mole $Cp^o/R = -0.366755 + 0.0587816\ T - 2.42517E\text{-}5\ T^2$

4) Mole $Cp(l) = 559.336 - 1.86259\ T + 0.2258292E\text{-}2\ T^2$, (kJ/kgmol, K)
(assumed same as o - Cresol)

5) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

6) Viscosity, vs: $\log vs\ (\text{cp}) = 1785.6\ (1/T - 1/370.75)$

A6 - p - Cresol, C_7H_8O

1) Molecular Weight, M — 108.14

2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 704.6, 50.8, 318.0, 0.246

3) Acentric factor; dipole moment — $\omega = 0.515$, $\mu = 1.60$ D

4) T_{tp}(K), T_b (K) — 308.7, 475.1

5) At 293.16 K, ρ_l (g/cm^3) — 1.035

6) At 298.16 K

	Cp(l)	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	55.29	29.75 (cals/gmol, K)	83.09	11.34	-29.97 (kcal/gmol)	-7.38
b)	231.4	124.5 (kJ/kgmol, K)	347.8	47,469	-125,454 (kJ/kgmol)	-30,893

Equations

1) Liquid volume, $V_l = 15.0901\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Vapor pressure: $\ln P\ (\text{torr}) = 16.1989 - 3479.39/(T - 111.3)$

$\ln P\ (\text{atm}) = 8.90052 - 2416.26/T - 861641/T^2$

3) Mole $Cp^o/R = 0.105993 + 0.0572001\ T - 2.31614\text{E-}5\ T^2$

4) Mole $Cp(l) = 559.336 - 1.86259\ T + 0.2258292\text{E-}2\ T^2$, (kJ/kgmol, K)
(assumed same as o - Cresol)

5) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

6) Viscosity, vs: $\log vs\ (\text{cp}) = 1826.9\ (1/T - 1/372.68)$

A7 - 2,3 - Xylenol, $C_8H_{10}O$

1)	Molecular Weight, M	122.17
2)	T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c	722.9, 48.0, 310.0, 0.251
3)	Acentric factor; dipole moment	$\omega = 0.464$, $\mu = 1.80$ D
4)	T_{tp}(K), T_b (K)	348.2, 491.2
5)	At 298.16 K, ρ_1 (g/cm^3)	1.1695

6) At 298.16 K

	$Cp(1)$	Cp°	S°	ΔH^v	ΔH_f°	ΔG_f°
a)	62.34	25.66	93.51	11.33	-37.57	-9.69
	(cals/gmol, K)			(kcal/gmol)		
b)	261.0	107.4	391.4	47,427	-157,268	-40,562
	(kJ/kgmol, K)			(kJ/kgmol)		

Equations

1) Liquid volume, $V_1 = 15.0581\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Vapor pressure: $\ln P\ (\text{torr}) = 17.2878 - 4274.42/(T - 74.09)$

$\ln P\ (\text{atm}) = 9.53837 - 3239.93/T - 657234/T^2$

3) Mole $Cp^\circ/R = 5.40946 + 8.73061E{-}2T - 7.24616E{-}5\ T^2 + 2.49691E{-}8\ T^3$

4) Mole $Cp(1) = 145.723 + 0.386692\ T$, (kJ/kgmol, K)

5) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$

6) Viscosity, vs: $\log vs\ (\text{cp}) = 1785.6\ (1/T - 1/370.75)$

A8 - Hydrogen, H_2

1) Molecular Weight, M — 2.016
2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 33.27, 12.79, 65.001, 0.292
3) Acentric factor; dipole moment — $\omega = -0.22$, $\mu = 0.0$ D
4) T_{tp}(K), T_b (K) — 14.06, 20.40
5) At 20.46 K, ρ_l (g/cm^3) — 0.0709
6) At 298.16 K

	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	6.89	31.21	0.216	0	0
	(cals/gmol, K)			(kcal/gmol)	
b)	28.85	130.65	903.74	0	0
	(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_l = 0.955\ (5.7 + 3T_r)$, ($cm^3$/gmol)
2) Liquid density, $\rho_l = 1.601406 + 1.1026\ [1 + (1 - T/33.25)^{0.272}]$, ($kgmol/m^3$)
3) Vapor pressure: $\ln P\ (torr) = 14.7996 - 232.321/(T - 8.08)$

   $\ln P\ (atm) = 2.06561 + 82.9148/T - 2604.56/T^2$
4) Mole $Cp^o/R = 3.44471 + 8.38932E{-5}\ T + 9.16277E{-8}\ T^2$
5) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$
6) Surface tension, $\sigma = 0.5363E{-2}\ (1 - T_r)^{1.074}$, (N/m)
7) Viscosity, vs: $\log vs\ (cp) = 13.82\ (1/T - 1/5.39)$

APPENDIX B: REACTANT AND PRODUCT PRICES

Reactants: [8]

Substance	Basis	Price
Phenol	synthetic, tank cars	\$ 0.46/lb
Methanol	synthetic, barges	0.49/gal 0.074/lb
Benzene	industrial, barges	1.15/gal 0.156/lb
n-hexane	industrial, tank cars	0.74/gal 0.134/lb
	95%, tank cars	0.85/gal 0.154/lb
n-heptane	industrial, tank cars	0.68/gal 0.179/lb
	95%, tank cars	0.95/gal 0.166/lb

Products: [8]

Substance	Basis	Price
o-Cresol	99% pure, bulk	\$ 0.58/lb
m-Cresol	95-98%, drums	1.71/lb
	tanks	1.65/lb
p-Cresol	bulk	1.30/lb
m,p-Cresol	bulk	0.82/lb
mixed xylenols	bulk	0.58/lb

Gases (current Gulf Coast prices):

Substance	Mi	$\$/10^6$ Btu	\$/lb
Hydrogen (H_2)	2.016	1.30	0.0792
Methane (CH_4)	16.042	1.30	0.0310

APPENDIX C: PLANT UTILITIES & COST

(Operating hours/y: Reaction Section = 2500; Separation Section = 8400)

Reaction Section

Utility	Amount	Unit Cost	$/h	$/y
1) CW	2.103E4 lbm/h 2.519E3 gal/h	$0.10/1000 gal	0.2519	6.298E2
2) Steam, 500 psia	1.784E3 lbm/h	$2.20/1000 lbm	3.925	9.812E3
3) Electrical power,* a) pumps	1.587E4 kJ/h	$0.041/kWh	0.1807	4.519E2
b) lights, instru., comp.	1.587E4 kJ/h	$0.041/kWh	0.1807	4.519E2
		(for 2500 h)	$4.538/h	$11,345/y

Separation Section

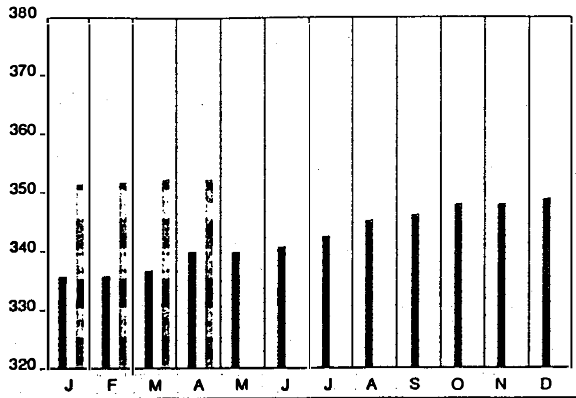
Utility	Amount	Unit Cost	$/h	$/y
1) CW	9.197E4 lbm/h 1.102E4 gal/h	$0.10/1000 gal	1.102	9.257E3
2) Steam, 500 psia	3.751E3 lbm/h	$2.20/1000 lbm	8.252	6.932E4
3) Electrical power, * a) pumps	6.953E3 kJ/h	$0.041/kWh	0.07919	6.652E2
b) lights, instru., comp.	6.953E3 kJ/h	$0.041/kWh	0.07919	6.652E2
		(for 8400 h)	$9.512/h	$79,907/y

$0.09125E6/y

* plant generated

1988 1989

CHEMICAL ENGINEERNG PLANT COST INDEX

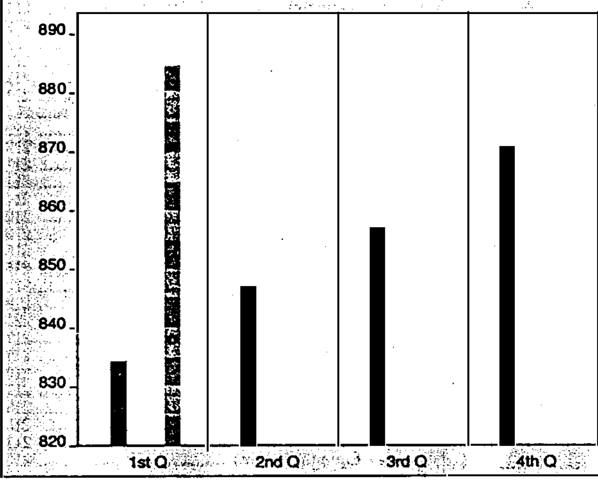


(1957-59 = 100)	Apr.'89 Prelim.	Mar.'89 Final	Apr.'88 Final
CE INDEX	**354.2**	**354.2**	**340.1**
Equipment	391.0	390.7	369.4
Heat exchangers & tanks	372.6	372.5	352.8
Process machinery	360.4	360.5	342.6
Pipe, valves & fittings	463.6	463.5	427.5
Process instruments	351.9	353.0	338.9
Pumps & compressors	479.4	478.4	443.3
Electrical equipment	284.4	285.8	266.2
Structural supports & misc.	375.2	372.5	373.0
Construction labor	267.0	267.7	264.5
Buildings	325.9	325.9	318.3
Engineering & supervision	341.3	341.4	343.5

Annual Index

1983 = 316.9
1984 = 322.7
1985 = 325.3
1986 = 318.4
1987 = 323.8
1988 = 342.5

MARSHALL & SWIFT EQUIPMENT COST INDEX



(1926 = 100)	1th Q 1989	4th Q 1988	1st Q 1988
M & S Index	**884.7**	**869.5**	**835.3**
Process industries, average	902.7	889.1	851.4
Cement	898.9	884.2	851.7
Chemical	892.9	879.1	840.0
Clay products	884.6	870.3	837.7
Glass	839.1	824.6	790.4
Paint	902.5	888.4	849.6
Paper	850.5	837.7	801.7
Petroleum products	938.7	926.0	889.4
Rubber	956.8	942.8	904.6
Related industries,			
Electrical power	869.6	843.7	818.4
Mining, milling	905.5	886.0	855.1
Refrigerating	1046.2	1030.1	986.0
Steam power	888.7	872.0	834.4

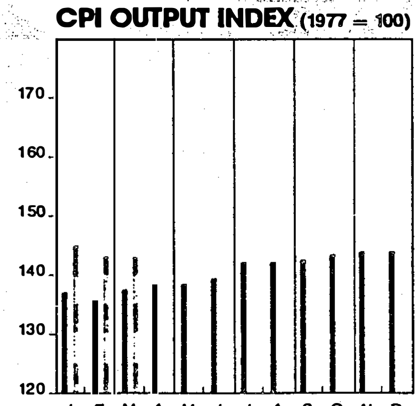
Annual index

1983 = 760.8
1984 = 780.4
1985 = 789.6
1986 = 797.6
1987 = 813.6
1988 = 852.0

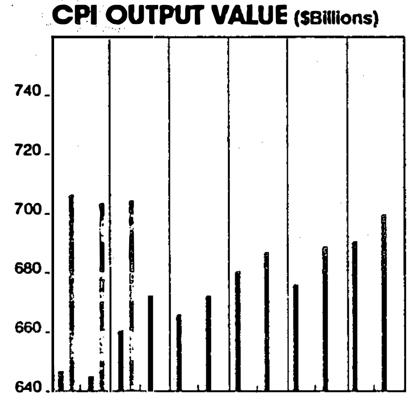
CURRENT BUSINESS INDICATORS

	LATEST	PREVIOUS		YEAR AGO
CPI output index (1977 = 100)*	Mar. '89=144.0P	Feb. '89=143.8R	Jan. '89=145.0R	Mar. '88=137.4
CPI value of output, billion $ †	Mar. '89=703.1P	Feb. '89=704.1R	Jan. '89=708.6R	Mar. '88=661.7
CPI operating rate, %	Mar. '89=87.7P	Feb. '89=88.0R	Jan. '89=89.0R	Mar. '88=87.5
Construction cost index (1913 = 100)	May. '89=4572.3	Apr. '89=4570.9	Mar. '89=4567.6	May. '88=4493.2
Producer prices, industrial chemicals (1982 = 100) ‡	Apr. '89=117.8	Mar. '89=116.9	Feb. '89=117.6	Apr. '88=103.3
Index of industrial activity (1967 = 100)	May 6, '89=176.8	Apr. 29, '89=177.2	Apr. 15, '89=176.7	May 8, '88=171.5
Hourly earnings index, chemical & allied products (1977 = 100)	Apr. '89=200.1	Mar. '89=200.9	Feb. '89=200.4	Apr. '88=195.4
Productivity index, chemicals & allied products (1977 = 100)	Mar. '89=159.2	Feb. '89=157.0	Jan. '89=158.5	Mar. '88=149.5

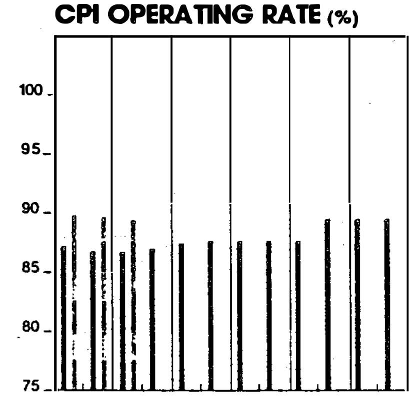
CPI OUTPUT INDEX (1977 = 100)



CPI OUTPUT VALUE ($Billions)



CPI OPERATING RATE (%)



*To convert to 1967 = 100 base, multiply by 1.675. †Revised as of Jan. 1987 — multiply values from Jan 1982 to Jan. 1987 by 0.9586 to convert to values starting with Jan. 1987; ‡To convert to 1967 = 100 base, multiply by 3.524; §To convert to 1967 = 100 base, multiply by 3.5241. P = Preliminary; R = Revised. For an explanation and additional information call: (212) 512-6931 or (212) 512-6793

SYMBOLS & NOMENCLATURE

upper case (chemical element symbols not included)

A	heat transfer area
C, C_o	plant capital cost, correlation constant
$C_p(l)$, C_p^o	liquid heat capacity, perfect gas state heat capacity
CX	cresol-xylenol fractionator
F, F_o	fresh feed, base case fresh feed
ΔG_f^o	Gibbs free energy of formation
G, L	gas mole flow rate, liquid mole flow rate
Gmax	maximum gas flow rate
ΔH_f^o, ΔH^v	enthalpy of formation, enthalpy of vaporization
Ic, Inc, PI	cost index, income, plant income
LK, HK	light key, heavy key components
Mi	molecular weight
MC	material of construction
OCX	o-cresol xylenol fractionator
P, P_c	pressure, critical pressure
PF	primary fractionator
POC, Top	plant operating cost, total operating cost
Q, Qsolar	heat transfer rate, solar energy input
Re	Reynolds number
REAC, Rm	reactor, raw material cost
S^o	perfect gas state entropy
Sf, SS, TS	scale factor, shell-side, tube-side
T_b, T_c, T_{tp}	n-boiling point, critical temperature, triple point
ΔT_{LM}	log-mean temperature difference
U	overall heat transfer coeficient
V, $V(l)$, V_c	volume, liquid volume, critical volume
Vmax	maximum vapor velocity
Xi, Yi	liquid and vapor mole fractions
Z, Z_c	compressibility factor, critical value

lower case

h	individual heat transfer coefficient
vs	liquid viscosity

Greek

μ	dipole moment
ρ_G, ρ_L	gas density, liquid density
σ	surface tension
ω	acentric factor

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16. Abstract (Limit: 200 words)
This is the second of two reports that compare the manufacture of cresols and xylenols using two processes--a conventional catalytic process and a solar photothermal catalytic process--to determine the relative process economics. This report presents results of a process evaluation for the photothermal catalytic process. (The first report, Synthesis of Cresols and Xylenols from Phenol and Methanol, evaluates the conventional catalytic process.) An arbitrary base case plant size (fresh feed) of about 7.06 million kg/y (15.6 million lbm/y) was chosen and then scaled to a breakeven size. The evaluation indicates that the breakeven capacity is only about 24% of the base case and about the same percentage of the conventional catalytic process evaluated in the first report. Assuming the total capital cost would double, which is unlikely, when the solar equipment is included, the overall conclusion in favor of the photocatalytic process would not change.

17. Document Analysis
a. Descriptors
Photothermal catalytic; cresols; xylenols; benzene; methanol; synthesis

b. Identifiers/Open-Ended Terms

c. UC Categories
248

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