NREL/TP-253-4276 • UC Category: 248 • DE91002141

NREL/TP--253-4276

DE91 002141

Synthesis of Cresols and Xylenols from Phenol and Methanol

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(formerly the Solar Energy Research Institute)
1617 Cole Boulevard
Golden, Colorado 80401-3393
A Division of Midwest Research Institute
Operated for the U.S. Department of Energy
under Contract No. DE-AC02-83CH10093

Prepared under Subcontract No. XX-7-07028-1

April 1992

Printed in the United States of America
Available from:
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

Price: Microfiche A01
Printed Copy A03

Codes are used for pricing all publications. The code is determined by the number of pages in the publication. Information pertaining to the pricing codes can be found in the current issue of the following publications which are generally available in most libraries: *Energy Research Abstracts (ERA)*; *Government Reports Announcements* and Index (*GRA* and I); *Scientific and Technical Abstract Reports (STAR)*; and publication NTIS-PR-360 available from NTIS at the above address.

• EXECUTIVE SUMMARY •

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

This report is the first of two reports, the one presenting the results of a process study and evaluation for manufacturing the products by a conventional catalytic process. The process generally favored in the US is the vapor-phase methylation of phenol using a high mole ratio of methanol over a solid acidic catalyst. The research reported in the literature was used as a basis for sizing the reaction system. The major pieces of equipment are: 1- reactor, 1- process heater, 4-fractionators, 11-heat exchangers, 9-pumps, and 4-storage tanks.

At the outset of calculations the plant size for break-even economics was not known; therefore an arbitrary base case plant size (fresh feed) of approximately 7 million kg/y (15.3 million lbm/y) was chosen, and then escalated to break-even size. Subsequent calculations indicated the following important numbers:

BASE CASE:

1) Plant Size, fresh feed =7 E6 kg/y, products =	5.54 E6 kg/y
2) Plant Capital Cost	$ 2.022 E6
3) Plant Operating Cost (POC)	$ 7.015 E6 /y
4) Plant Income (PI)	$ 6.413 E6 /y
5) PI/POC	0.9142

BREAK-EVEN CASE:

1) Plant Size, fresh feed = 12.80 E6 kg/y, products = 10.22 E6 kg/y	
2) Plant Capital Cost	$ 2.919 E6
3) Plant Operating Cost and Income	$11.83 E6/y

Conclusion: assuming that an owner chemical company could obtain a fair share of the market, it is estimated that a profitable operation would result for a plant size greater than 12.80 E6 kg/y of fresh feed.

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. INTRODUCTION .

This report is the first of two reports 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 processes, and the relative process advantages and economics.

The purpose of this report is to present the work accomplished on sizing and costing a conventional catalytic process to produce cresols and xylenols from phenol and methanol. One of the standard chemical process references, Faith, Keyes and Clark [1], reviews the different processes for cresols and xylenols, and states the following: *"The process generally favored in the United States is the vapor phase methylation of phenol with methanol over a solid acidic catalyst. At higher temperatures ortho-methylation is the predominant reaction, giving o-cresol and 2,6-xylenol as major products. As the temperature is raised above 350 C, meta- and paramethylation become more pronounced, leading to formation of m- and p-cresol, the various xylenols other than 2,6-isomer, and polymethylphenols".*

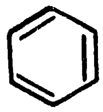
Hence the vapor phase catalytic methylation process was chosen for economic evaluation. No process configuration, sizing, and costing were available; therefore, the necessary calculations were made to obtain the details of the process.

1.00 PRODUCTION AND PRODUCT MARKET

At the outset the reader should become familiar with the structures of the product compounds, in order to visualize the synthesis chemistry starting with phenol and methanol. In the catalytic reaction, which is conducted with a large excess of methanol, the phenol provides the benzene ring structure and the methanol the methylation groups.

The reactants:

phenol
C_6H_5OH



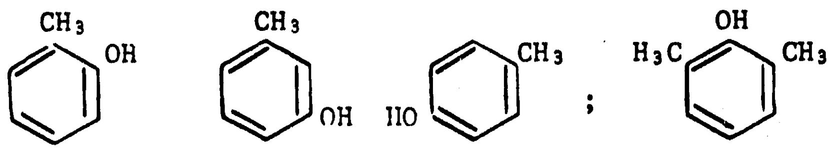
M=94.113 ;

methanol
M=32.042

H_3C-OH

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 primerily 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] is shown in Table 1; it will be noted that the total cresol and xylenol consumptions were approximately equal, 208 vs. 218 million pounds per year in 1986.

Table 1. Consumption of Cresols and Xylenols
(millions of pounds per annum, 1986)

compound	USA	w.Europe	Japan	(total)
1) o-cresol	10	47-49	15	(72-74)
2) m-cresol	5-6	3	25	(33-34)
3) p-cresol	18-19	24	18	(60-61)
4) m,p-cresol	10	0	31	(41)
5) xylenols	110	57	51	(218)
6) cresylic acid	24	0	14	(38)
Totals	177-179	131-133	154	(462-466)

The U.S. price history of the products is shown in Table 2; more details about current reactant and product prices are given in Appendix B.

Table 2. U.S. Prices ($/lb.) for Cresols and Xylenols

	cresols					
year	ortho-	meta-	para-	m,p-	2,6-xyl	mix-xyl
1960	0.14	0.60	0.49	0.20		
1970	0.165	0.60	0.42	0.175		
1980	0.555	0.93	1.25	0.70		
1985	0.75	1.65	1.00	0.61		
1987	0.57	1.00	1.15	0.61	0.80	0.58
1989	0.58	1.65	1.30	0.82	(0.80)	(0.58)

2.00 PROCESS DESCRIPTION AND DESIGN BASIS

The reader is referred to the flow diagram, Figure 1 (p 5), which was produced, along with certain process calculations, using CHEMCAD II-Process Flowsheet Simulator [3]. This computer simulator is currently in use as a tool in chemical engineering design courses, as well as by chemical and refining companies for preliminary process designs and cost estimates. A complete mass balance at key points through the process as well as process temperatures are shown.

The approximate overall stoichiometry for the process is,

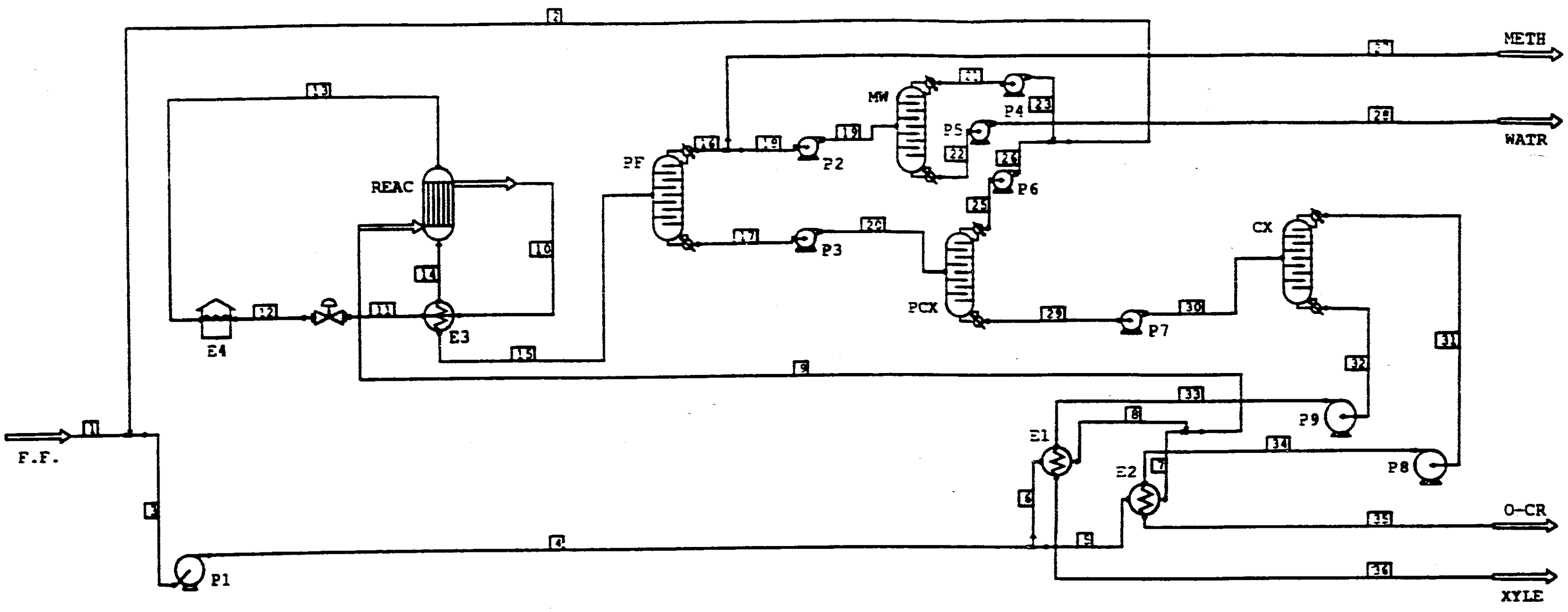
$$C_6H_5OH + 1.432\ CH_3OH \rightarrow 0.6998\ C_7H_8O + 0.2539\ C_8H_{10}O + 1.208\ H_2O + 0.0467\ CH_4 + (3.6\%\ \text{other fragments}) \quad (1)$$

The reaction is exothermic in the amount of -41,860 kJ/kgmole of phenol, with a per reactor pass phenol conversion of 58.3%.

The process flow, fresh feed to final products, proceeds as follows: fresh feed stream 1, consisting of 1.432:1 mole ratio of methanol to phenol at 25 C joins the recycle stream 2. The composite stream 3, 6:1 methanol to phenol, passes through heat exchangers E1 and E2, then through the shell side of the reactor, E3, and the process heater, E4 where it is vaporized before entering the reactor at ~420 C. The reactor design is based on data reported by Sumitomo Chemical Company [4]. The reactor output stream 14, consisting of cresols, xylenols, water, methane and unconverted phenol and methanol, flows to the primary fractionator (PF) as stream 15, where the water, methanol, and methane are separated from the other components. The methane is flashed from the partial condenser on the PF.

The methanol plus water stream 18 flows to the MW fractionator for separation, the methanol being recycled. Stream 17 from the PF is pumped to the phenol-cresol-xylenol (PCX) fractionator, which separates the phenol for recycle with the methanol as stream 2. Final fractionation of the cresol-xylenol stream 29 is accomplished in the CX fractionator, with o-cresol being taken off as the tops product 35, and mixed xylenol-cresols as bottoms stream 36.

Heat exchange is accomplished where possible in order to reduce the need for purchased fuel; cooling water and steam are the heat media, and electric power is required for the pumps.



Component	M.W.	1	2	15	19	20	23	26	30	27	28	35	36
		streams and flow rates, kg/h											
PHENOL	94.114	556.54	384.60	392.45	0.0000	392.45	0.0000	384.60	7.8489	0.0000	0.0000	7.8489	0.0000
METHANOL	32.042	270.19	1652.3	1688.3	1676.6	9.1892	1643.1	9.1893	0.0000	2.4284	33.533	0.0000	0.0000
O-CRESOL	108.14	0.0000	0.0000	437.97	0.0000	437.97	0.0000	0.0000	437.96	0.0000	0.0000	416.06	21.898
M-CRESOL	108.14	0.0000	0.0000	1.6221	0.0000	1.6221	0.0000	0.0000	1.6221	0.0000	0.0000	0.0000	1.6221
P-CRESOL	108.14	0.0000	0.0000	1.6221	0.0000	1.6221	0.0000	0.0000	1.6221	0.0000	0.0000	0.0000	1.6221
WATER	18.015	0.0000	4.9580	131.78	129.01	2.6357	2.3223	2.6357	0.0000	0.13401	126.69	0.0000	0.0000
METHANE	16.043	0.0000	0.44245	4.7616	0.44245	0.0000	0.44245	0.0000	0.0000	4.3676	0.0000	0.0000	0.0000
XYLENOL	122.17	0.0000	0.0000	180.81	0.0000	180.81	0.0000	0.0000	180.81	0.0000	0.0000	0.0000	180.81
OTHERS	-	0.0000	0.0000	29.705	0.0000	29.705	0.0000	0.0000	29.705	0.0000	0.0000	0.0000	29.705
		826.73	2042.3	2869.0	1806.1	1056.0	1645.9	396.43	659.57	6.9300	160.23	423.91	235.66
T (C)		25	67.4	147	60	162	64.5	180	200	60	66	70	70

Figure 1. PROCESS FLOW DIAGRAM

The major pieces of equipment are:

1- process heater; 1- reactor; 4- fractionators;

11- heat exchangers; 9- pumps, and 4- storage tanks.

Although one reactor is shown on Figure 1, two reactors are proposed in order to increase operational flexibility, as discussed in the next section of this report.

At the outset thr break-even capacity is not known. However, the functional form of the scaling equations is known, but not the constants in the equations; these must be determined from one case. Based on market demand and typical plant size, the following design basis was chosen for the base case:

Fresh Feed	6.94 million kg/y = 15.3 million lbm/y
Operating time	8400 h/y (downtime 360 h/y)
Cresols	3.49 million kg/y = 7.71 million lbm/y
Xylenols	1.52 million kg/y = 3.35 million lbm/y

3.00 CHEMICAL REACTION/REACTOR SECTION

The plant has two major sections: a Reaction Section and a Separation Section. The former 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 2; the stream numbers, temperatures, pressures, and heat exchanger Q-values are shown on the diagram. Table 3 presents mass balance and composition values for streams 1, 2, 3 to 11, and 14.

The flow proceeds as follows. Recycle stream 2 is joined by the fresh feed stream 1 to produce the composite feed stream 3, which is pumped by P1 through heat exchangers E1 and E2. The pump pressure is 405 psia, selected to provide sufficient pressure drop through the equipment (E1, E2, REAC, and E3) and insure liquid phase up to the control valve at the entrance to the process heater E4. The chemical reaction is exothermic, hence in order to remove the heat evolved and maintain the reactor effluent temperature at a reasonable level, liquid stream 9 flows through the shell side of the reactor, exiting at 83 C as stream 10. Stream 10 in turn flows through the economizer E3 to the control valve which partially releases the pressure before entering process heater E4, where complete vaporization of the stream occurs. The gas mixture stream 13, mainly phenol and methanol, enters the reactor at 420 C and 30 psia.

The exothermic catalytic reaction between phenol and methanol takes place in the reactor, which is of shell-and-tube design; the catalyst pellets being packed inside the tubes. Two

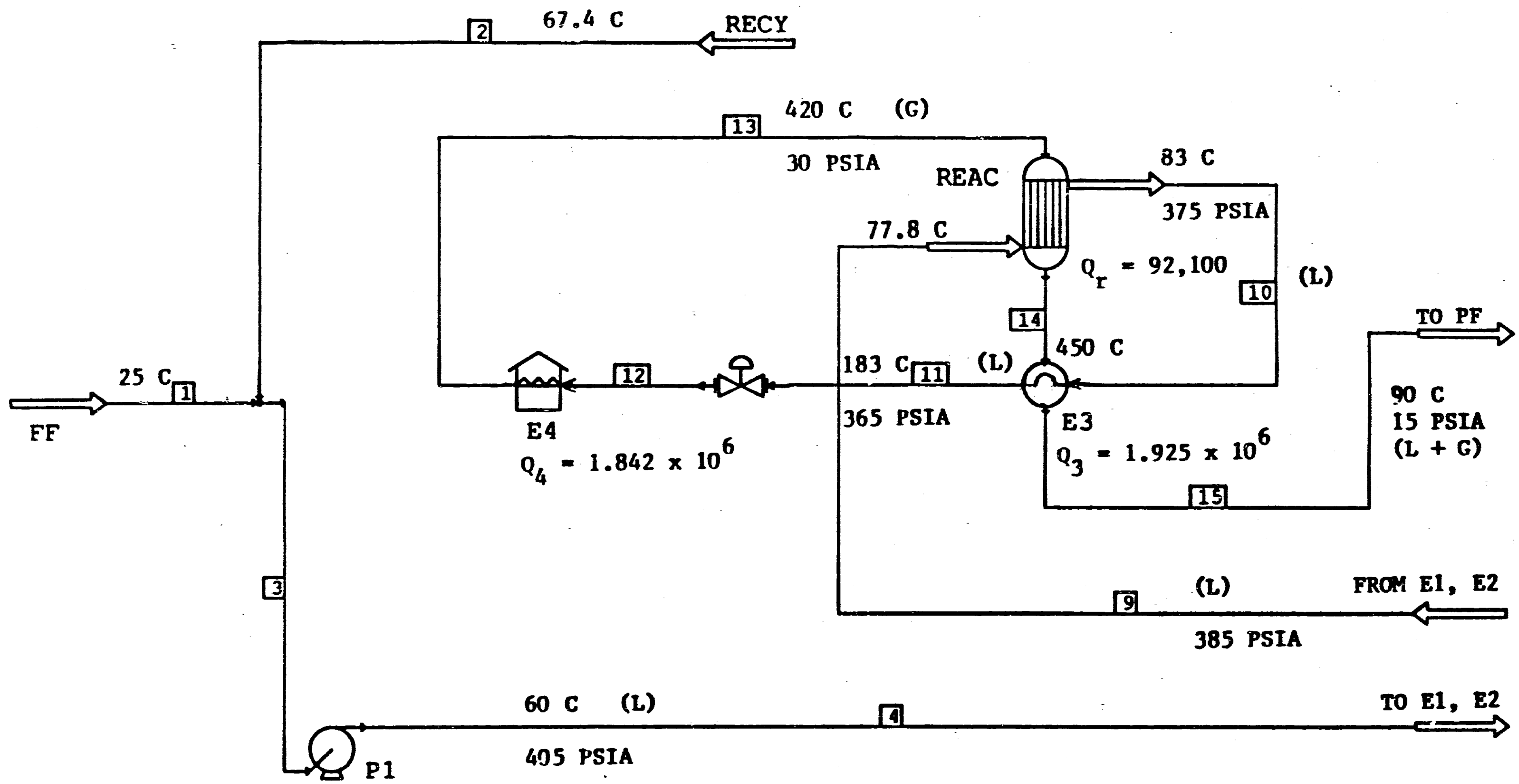


Figure 2. REACTION SECTION
(Note: Q-values are kJ/h)

Table 3. REACTION SECTION MASS BALANCE & COMPOSITIONS

	streams:	1	2	3 to 11			14		
Comp	M_i	kg/h	kg/h	kg/h	kgmols/h	X_i	kg/h	kgmols/h	Y_i
C_6H_5OH	94.114	556.54	384.60	941.14	10.0000	0.1422	392.45	4.1699	0.0595
CH_3OH	32.042	270.19	1652.3	1922.49	60.0000	0.8535	1688.3	52.6902	0.7524
C_7H_8O	108.14	-	-	-	-	-	441.21	4.0800	0.0583
H_2O	18.015	-	4.9580	4.9580	0.2750	0.0039	131.78	7.3150	0.1045
CH_4	16.043	-	0.44245	0.44245	0.0760	0.0004	4.7616	0.2968	0.0042
$C_8H_{10}O$	122.17	-	-	-	-	-	180.81	1.4800	0.0211
Others	-	-	-	-	-	-	29.705	-	-
		826.73	2042.3	2869.0	70.351	1.0000	2869.0	70.032	1.0000

heat transfer phenomena occur in the reactor: a) -as the heat is released by reaction inside the pellets it flows transversly by conduction and convection to the tube surface, and b) -then through the tubes to the the liquid on the shell side. Detailed calculations were carried out on the reactor, first assuming that a single-reactor would be used, and second assuming a two-reactor case. Table 4 summarizes the reactor design parameters for both cases.

The reactor effluent stream 14 at 450 C flows through E3 where the temperature is reduced and partially condensed (to approximately 35 mole% liquid), and thence as stream 15 to the primary fractionator (PF) to begin the separation and recycle sequence.

Table 4. REACTOR SPECIFICATIONS

Item	Single-Reactor Case	Two-Reactor Case (per reactor)
1) Type	Fixed bed, shell and tube, catalyst pellets inside tubes	
2) Catalyst	CeO_2/SiO_2, 3 x 3 mm pellets	
	mass = 137.6 kg	68.8
	volume = 0.3112 m^3	0.1556
3) Tubes	15	7
	4.026" id. x 9' long, stainless steel	
	volume = 0.4668 m^3	0.2334
4) Shell	32" id. carbon steel	24" id.
	3.5" tube clearance	2.5"
	36" baffle spacing	36"
5) Space velocity	0.5113 (kgmols/h,kg catalyst)	
6) Q (exo)	92,100 kJ/h	46,050
7) Re (tube)	861.3	927.5
8) Re (shell)	1894	1043
9) ΔT_{Lm}, deg	254.5	
10) h (tube)	58.45 (kJ/m^2h K)	62.16
11) h (shell)	31.24 "	33.61
12) U (overall)	20.36 "	21.81
13) A (heat transfer)	12.76 m^2	5.956
14) Estimated Cost (per reactor)	$13,644	$7745

4.00 EQUIPMENT SIZING AND COST

Specifications and costs for the individual pieces of equipment are presented in Tables 6-9 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 D) was calculated by, I(1974) = 202.5, I(1989) = 391.0, giving I_c = 391.0/202.5 = 1.931.

The costs by catagory are summarized in Table 5, as follows.

Table 5. SUMMARY OF EQUIPMENT COSTS
(fresh feed = 6.94 million kg/y = 15.3 million lbm/y)

catagory	number	Cost ($)
1) Reactors	(2)	15,490
2) Heat exchangers, incld process heater	(12)	221,600
3) Distillation columns	(4)	141,200
4) Accumulators	(4)	32,000
5) Pumps with spares	(9)	24,400
6) Storage tanks	(4)	119,200
		(553,890)
7) Process Instruments & Controls (15%)		83,100
8) Computer (data logging & control)	(1)	100,000
9) Catalyst, initial charge	(1)	1,000
Total Equipment		$738,000

Table - HEAT EXCHANGER SUMMARY

	Duty kJ/h	Fluids TS/SS	T_{in} (C)	T_{out}	ΔT_{Lm} U Area	MC	Estimated cost
E1 Feed Preheater #1	0.0991E6	Feed CX Top	60 190	77.8 70	42.27 K 250 9.45 m^2 = 102 ft^2	304 SS CS	$ 2018
E2 Feed Preheater #2	0.05465E6	Feed CX Btm	60 212	77.8 70	47.82 250 4.57 = 49.19	304 SS CS	$ 1938
E3 Economizer	1.925E6	Feed (L) RX Effluent	83 450	183 90	71.4 250 107.8 = 1160	304 SS CS	$34,439
E4 Process Heater	1.842E6	Feed (L+G) Combustion Gas	183	420		304 SS Refractory/CS	$15,738
E5 PF Col. Condenser	3.910E6	CW PF Ovhd	32 62.15	54 62.15	16.8 7560 30.79 = 331.3	304 SS CS	$25,251
E6 PF Col. Reboiler	0.5933E6	Steam PF Btm	180 162	180 162	42 1430 23.05 = 248.02	304 SS CS	$19,857

Table 6 - HEAT EXCHANGER SUMMARY (continued)

	Duty kJ/h	Fluids TS/SS	T_{in} (C)	T_{out}	ΔT_{Lm} U Area	MC	Estimated cost
E7 MW Col. Condenser	2.322E6	CW MW Ovhd	32 62.74	54 62.74	19.74 7560 15.56 = 167.4	304 SS CS	$14,468
E8 MW Reboiler	2.661E6	Steam MW Btm	100 66	100 66	34 1430 55.73 = 599.7	304 SS CS	$39,930
E9 PCX Condenser	2.681E6	CW PCX Ovhd	32 180	54 180	137.8 1675 11.62 = 125	304 SS CS	$10,169
E10 PCX Reboiler	2.767E6	Steam PCX Btm	242 200	242 200	42 1430 46.07 = 495.7	304 SS CS	$33,444
E11 CX Condenser	1.217E6	CW CX Ovhd	32 195	54 195	151.73 1675 4.79 = 51.52	304 SS CS	$ 6094
E12 CX Reboiler	1.224E6	Steam CX Btm	242 200	242 200	42 1430 20.38 = 219.3	304 SS CS	$18,262
						Total ($)	221,608

Table 7a. PF Distillation Column

Feed stream 15; overhead stream 18; bottoms stream 17

Parameter		Top of column	Bottom of column
Z, comp. factor		1	1
Temperature	C	62.15	162.04
Pressure	atm	1	1
Liq. density	kg/m^3	753.040	931.280
Gas density	kg/m^3	1.10	2.83
Gas av. mol. wt.		30.29	100.98
Liq.surface tension	dyn/cm	19.66	25.04
Feed flow	kg/h	2838.9	
Vapor fraction in feed		0.65	
Reflux ratio		0.72077	
Dist. flow	kg/h	1812.61	
Gas flow	kg/h	3119.08	934.07
Liq. flow	kg/h	1306.47	1960.36
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.01602	0.1157
Tray spacing	in.	18	18
K	ft/s	0.29	0.25
Vmax	m/s	3.1	1.9
Gmax	kg/hm^2	1.212E4	1.953E4
"Active" area	m^2	0.26	0.05
Calc. column dia.		0.60 m = 1.98 ft	

Condenser type		partial
Feed flow	kg/h	2838.9
Feed temperature	C	90
LK/HK		water/PhOH
Recovery of LK in overhead	%	98
Recovery of HK in overhead	%	0.001
Actual stages		9
Operating reflux ratio		0.7208
Feed stage		7 top down
Condenser duty	kJ/h	3.514E6
Reboiler duty	kJ/h	0.5933E6
Overhead temperature	C	62.2
Bottom temperature	C	162.0
Distillate flow	kg/h	1812
Bottom flow	kg/h	1026
Design pressure	psig	200
Column dimensions [d x h (s to s)]		2' id x 22'
MC		CS/304 SS
Estimated Cost		$10,300

Table 7b. MW Distillation Column

Feed stream 19; overhead stream 21; bottoms stream 22

Parameter		Top of column	Bottom of column
Z, comp. factor		0.9817	1
Temperature	C	64.74	65.97
Pressure	atm	1	1
Liq. density	kg/m^3	750.000	899.000
Gas density	kg/m^3	1.18	7.13E-1
Gas av. mol. wt.		32.00	19.84
Liq. surface tension	dyn/cm	18.99	33.22
Feed flow	kg/h	1806.16	
Vapor fraction in feed		1	
Reflux ratio		0.28	
Dist. flow	kg/h	1645.89	
Gas flow	kg/h	2106.74	186.36
Liq. flow	kg/h	460.85	346.63
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.00866	0.05238
Tray spacing	in.	18	18
K	ft/s	0.28	0.27
Vmax	m/s	2.1	3.2
Gmax	kg/hm^2	9022.15	8298.13
"Active" area	m^2	0.23	0.02
Calc. column dia.		0.57 m = 1.89 ft	

Condenser type		total
Feed flow	kg/h	1806
Feed temperature	C	35
LK/HK		MeOH/Water
Recovery of LK in overhead	%	98
Recovery of HK in overhead	%	1.8
Actual stages		14
Operating reflux ratio		0.2834
Feed stage		7 top down
Condenser duty	kJ/h	2.322
Reboiler duty	kJ/h	2.661E6
Overhead temperature	C	64.7
Bottom temperature	C	66
Distillate flow	kg/h	1646
Bottom flow	kg/h	160
Design pressure	psig	

Column dimensions [d x h (s to s)]	2' id x 30'
MC	CS/304 SS
Estimated Cost	$13,500

Table 7c. PCX Distillation Column

Feed stream 20; overhead stream 25; bottoms stream 29

Parameter		Top of column	Bottom of column
Z, comp. factor		0.9764	1
Temperature	C	180.37	199.16
Pressure	atm	1	1
Liq. density	kg/m^3	930.000	900.160
Gas density	kg/m^3	2.30	2.88
Gas av. mol. wt.		87.71	111.61
Liq. surface tension	dyn/cm	19.66	25.04
Feed flow	kg/h	1026.29	
Vapor fraction in feed		1	
Reflux ratio		12.0176	
Dist. flow	kg/h	396.424	
Gas flow	kg/h	5160.49	5260.74
Liq. flow	kg/h	4764.07	5890.60
$(L/G)\ (\rho_1/\rho_g)^{0.5}$		0.04592	0.06333
Tray spacing	in.	18	18
K	ft/s	0.29	0.28
Vmax	m/s	1.8	17.0
Gmax	kg/hm^2	1.465E4	1.758E5
"Active" area	m^2	0.35	0.03
Calc. column dia.		0.71 m = 2.32 ft	

Condenser type		total
Feed flow	kg/h	1026
Feed temperature	C	162.0
LK/HK		phOH/o-cresol
Recovery of LK in overhead	%	98
Recovery of HK in overhead	%	0.001
Actual stages		80
Operating reflux ratio		12.0176
Feed stage		60 top down
Condenser duty	kJ/h	2.681E6
Reboiler duty	kJ/h	2.7674
Overhead temperature	C	180
Bottom temperature	C	199
Distillate flow	kg/h	396.5
Bottom flow	kg/h	629.8
Design pressure	psig	200
Column dimensions [d x h (s to s)]		2.5' id x 130'
MC		CS/304 SS
Estimated Cost		$62,900

Table 7d. CX Distillation Column

Feed stream 30; overhead stream 31; bottoms stream 32

Parameter		Top of column	Bottom of column
Z, comp. factor		0.9764	1
Temperature	C	194.46	212.66
Pressure	atm	1	1
Liq. density	kg/m^3	930.000	900.160
Gas density	kg/m^3	3.186	3.017
Gas av. mol. wt.		107.84	120.27
Liq. surface tension	dyn/cm	19.66	25.04
Feed flow	kg/h	629.86	
Vapor fraction in feed		1	
Reflux ratio		5.844	
Dist. flow	kg/h	423.908	
Gas flow	kg/h	2901.23	2533.02
Liq. flow	kg/h	2477.32	1738.97
$(L/G)\ (\rho_L/\rho_g)^{0.5}$		0.04998	0.06260
Tray spacing	in.	24	24
K	ft/s	0.40	0.40
Vmax	m/s	2.1	2.2
Gmax	kg/hm^2	2.377E4	2.388E4
"Active" area	m^2	0.122	0.0106
Calc. column dia.		0.42 m = 1.363 ft	

Condenser type		total
Feed flow	kg/h	629.9
Feed temperature	C	199.2
LK/HK		o-cresol/m-cresol
Recovery of LK in overhead	%	95
Recovery of HK in overhead	%	0.001
Actual stages		70
Operating reflux ratio		5.844
Feed stage		55 top down
Condenser duty	kJ/h	1.217E6
Reboiler duty	kJ/h	1.244E6
Overhead temperature	C	195
Bottom temperature	C	200
Distillate flow	kg/h	423.9
Bottom flow	kg/h	206.0
Design pressure	psig	200
Column dimensions [d x h (s to s)]		2' id x 150'
MC		CS/304 SS
Estimated Cost		$54,500

Table 8. PUMP SUMMARY

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

Pump	Inlet stream	Capacity (gpm)	ΔP(psi)	BHP	Cost($)
P1	3	16	500	10.6	5679
P2	18	16	135	2.86	2581
P3	17	6	135	1.10	2080
P4	21	20	135	3.59	2712
P5	22	1	135	0.20	1910
P6	25	30	135	6.11	2990
P7	29	4	135	0.72	1937
P8	31	17	135	3.05	2591
P9	32	1.5	135	0.27	1914

Total $24,400

Table 9. STORAGE TANK SUMMARY

(Based on approxiamte 10-day storage time)

Tank	Substance	Density (kg/liter)	Capacity (U.S. Gallons)	MC	Estimated Cost(1988)
T1	Phenol	1.069	35,000	CS	$33,600
T2	Methanol	0.788	25,000	CS	29,900
T3	o-Cresol	1.041	27,000	CS	30,700
T4	Xylenol	1.158	25,000	CS	25,000

Total $119,200

5.00 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 10. Estimated Capital Cost
(fresh feed = 6.94 million kg/y = 15.3 million lbm/y)

Item	factor	$/1000
A. Equipment (Table 5)		738.0
B. Interconnecting piping, flanges, fittings, valves	(15% A)	110.7
C. Assembly and Installation of Equipment		
purchasing, materials, labor and supervision	(40% A)	295.2
foundations and structures	(30% A)	221.4
running pipe, steam tracing, insulation, painting	(20% A)	147.6
electrical	(10% A)	73.8
		(1586.7)
D. Design and Engineering	(8% A+B+C)	126.9
E. BASE SYSTEM COST (BSC)		1713.6
F. Contractors fee	(8% BSC)	137.1
G. Contingency	(10% BSC)	171.4
H. TOTAL INSTALLED PLANT COST		$ 2.022 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 [$F = 6.94 \times 10^6$ kg/y, Ic (1989) = 1.931] the equation becomes,

$$C(\$) = Co\ Ic\ F^{0.60} = (82.257)\ Ic\ F^{0.60}$$

which can be used as the capital cost scaling-equation for different size plants. For example, for a plant of $F = 14 \times 10^6$ kg/y the estimated cost is $ 3.081×10^6.

The estimated plant operating cost is presented in Table 11. It is assumed that the plant is a process unit within an existing chemical plant where necessary utilities and other services are available.

Table 11. Plant Operating Cost
(8400 operating h/y)

Item	$/y
1) Raw Materials (phenol, methanol, supplies, make-up catalyst)	5.214 E6
2) Operating labor & supervision (3-operators, 1-technician, 1/2 foreman, per shift)	0.5292
3) Utilities (nat'l gas, steam, cooling water, electric power)	0.2029
4) Maintenance & Repair (7% of capital cost/y)	0.1416
5) Plant overhead (75% operating labor) 0.3969	
6) Plant G/A (25% operating labor)	0.1323
7) Depreciation (15 y life, loan payment) 0.1348	
8) Interest on borrowed capital (10%/y, 15y, on declining balance)	0.2022
9) Taxes and Insurance (3% of capital cost/y)	0.0607
10) TOTAL OPERATING COST	$ 7.0146 E6
11) Unit COST of PRODUCTS SOLD (7.0146/11.134)	$0.6300 /lbm

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

6.00 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 12.

Table 12. Plant Income from Products

product	lbm/y	$/lbm	$/y
1) methane	80,882	0.0307	2484
2) o-Cresol	7.705 E6	0.58	4.469 E6
3) mixed Xylenols	3.348 E6	0.58	1.942 E6
4) Totals	11.134 E6		6.413 E6
5) Average unit income	($6.413/11.134)		$0.5760 /lbm

Comparing the average $/lbm income with the cost/lbm (Table 11) it is obvious that the base case is below break-even, and the capacity will have to be escalated to find the break-even point. The operating cost items in Table 11 can be written in equation form and programmed 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 13 presents a computer print-out for determination of the first-year break- even point, giving the following values:

1) Fresh Feed	12.80 E6 kg/y
2) Products	10.22 E6 kg/y
3) Capital Cost	$ 2.947 E6
4) Operating Cost & Income	$ 11.83 E6/y

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

Finally, the report provides the following evaluative conclusions for the process:

1. -a plant producing greater than approximately 22.5 million poounds per year would be a profitable venture.

Table 13. 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)
6940000

TABLE 2 - Profitability Analysis as f(plant capacity)

J	Sf	C($)	Rm($)	Top($)	Inc($)	Inc/Top
1	1.0000	2021953	5214000	7014555	6413000	0.9142
2	1.4409	2517418	7512968	9535126	9240634	0.9691
3	1.7291	2808433	9015562	11173807	11088761	0.9924
4	1.8012	2878070	9391210	11582645	11550792	0.9972
5	1.8372	2912470	9579035	11786954	11781809	0.9996
6	1.8444	2919318	9616599	11827806	11828011	1.0000
7	1.8732	2946601	9766859	11991190	12012824	1.0018
8	1.9452	3014086	10142507	12399454	12474856	1.0061
9	2.0173	3080578	10518156	12807454	12936888	1.0101
10	2.1614	3210777	11269453	13622712	13860952	1.0175

Out of Data
END OF CALCULATION (7-10-89)

2. -the configuration of the process indicates the equipment complexity, which extends to the capital investment required.

3. -the major item of operating cost is raw materials (feedstock) -- primarily phenol cost.

4. -in total, the report provides a basis for comparison with a projected solar photo-catalytic process.

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APPENDIX A - PHYSICAL & THERMODYNAMIC PROPERTIES

A1 - Phenol, C_6H_5OH

1) Molecular Weight, M — 94.113
2) T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c — 694.3, 60.5, 229.0, 0.244
3) Acentric factor; dipole moment — $\omega = 0.426$, $\mu = 1.60$ D
4) T_{tp}(K), T_b (K) — 315.7, 455.0
5) At 298.16 K, ρ_l (g/cm^3) — 1.071
6) At 298.16 K

	$Cp(l)$	$Cp°$	$S°$	ΔH^v	$\Delta H_f°$	$\Delta G_f°$
a)	46.94	24.75	75.43	10.90	-23.03	-7.860
		(cals/gmol, K)			(kcal/gmol)	
b)	196.5	103.6	315.7	45,627	-96,404	-32,902
		(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_l = 12.607\ (5.7 + 3T_r)$, ($cm^3$/gmol)
2) Liquid density, $\ln \rho_l = 0.34854 + 1.13438\ [1 + (1 - T/0.6942E3)^{0.3212}]$, ($kgmol/m^3$)
3) Vapor pressure: $\ln P\ (torr) = 17.2917 - 4027.98/(T - 76.701)$
   $\ln P\ (atm) = 9.76704 - 2913.8/T - 697154/T^2$
4) Mole $Cp°/R = -\ 0.638357 + 0.0510768\ T - 0.227204E\text{-}4\ T^2$
5) Mole $Cp(l) = 101.961 + 0.31714\ T$, (kJ/kgmol, K)
6) $\Delta H^v = RT^2\ \Delta Z\ (d \ln P/dT)$
7) Surface tension, $\sigma = 0.0745\ (1 - T_r)^{1.0767}$, (N/m)
8) Viscosity, vs: $\log vs\ (cp) = 1405.5\ (1/T - 1/370.07)$

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	ω = 0.5656, μ = 1.70 D
4)	T_{tp}(K), T_b (K)	175.7, 337.8
5)	At 293.16 K, ρ_l (g/cm^3)	0.792

6) At 298.16 K

	Cp(l)	Cp°	S°	ΔH^v	ΔH_f°	ΔG_f°
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, $V_l = 5.4628\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Liquid density, $\ln \rho_l = 0.18706 + 1.62055\ [1 + (1 - T/0.51263E3)^{0.17272}]$, ($kgmol/m^3$)

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 $Cp^\circ/R = 1.85019 + 0.0124255\ T - 3.49129E{-6}\ T^2$

5) Mole $Cp(l) = -39.9665 + 0.787208\ T$, (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: $\log vs\ (cp) = 555.3\ (1/T - 1/260.64)$

APPENDIX A (continued)

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_1 (g/cm^3) — 1.048

6) At 298.16 K

	Cp(1)	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, $V_1 = 14.9288\ (5.7 + 3T_r)$, ($cm^3$/gmol)

2) Liquid density, $\ln \rho_1 = 0.58912 + 1.18685\ [1 + (1 - T/0.69755E3)^{0.3099}]$, ($kgmol/m^3$)

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 $Cp(1) = 559.336 - 1.86259\ T + 0.2258292E\text{-}2\ T^2$, (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°	S°	ΔH^v	$\Delta H_f°$	$\Delta G_f°$
a)	18.02	8.03 (cals/gmol, K)	45.11	9.717	-57.8 (kcal/gmol)	-54.64
b)	75.4	33.6 (kJ/kgmol, K)	188.8	40,675	-241,951 (kJ/kgmol)	-228,723

Equations

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: $\ln P\,(\text{torr}) = 18.3036 - 3816.44/(t - 46.13)$

   $\ln P\,(\text{atm}) = 11.6572 - 3761.58/T - 218339/T^2$
4) Mole $Cp°/R = 2.37293 + 0.0160161\,T - 7.40155E{-6}\,T^2$
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 — $\omega = 0.464$, $\mu = 1.80$ 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°	S°	ΔH^v	ΔH_f°	ΔG_f°
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 $Cp^\circ/R = -0.366755 + 0.0587816\ T - 2.42517E\text{-}5\ T^2$
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: $\log vs\ (cp) = 1785.6\ (1/T - 1/370.75)$

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 — ω = 0.515, μ = 1.60 D

4) T_{tp}(K), T_b (K) — 308.7, 475.1

5) At 293.16 K, ρ_1 (g/cm^3) — 1.035

6) At 298.16 K

	Cp(1)	Cp^o	S^o	ΔH^v	ΔH_f^o	ΔG_f^o
a)	55.29	29.75	83.09	11.34	-29.97	-7.38
	(cal./gmol, K)			(kcal/gmol)		
b)	231.4	124.5	347.8	47,469	-125,454	-30,893
	(kJ/kgmol, K)			(kJ/kgmol)		

Equations

1) Liquid volume, $V_1 = 15.0901\ (5.7 + 3T_r)$, ($cm^3$/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 $Cp^o/R = 0.105993 + 0.0572001\ T - 2.31614E\text{-}5\ T^2$

4) Mole $Cp(1) = 559.336 - 1.86259\ T + 0.2258292E\text{-}2\ T^2$, (kJ/kgmol, K)
(assumed same as o - Cresol)

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

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

A7 - Methane, CH_4

1)	Molecular Weight, M	16.042
2)	T_c (K), P_c (atm), V_c (cm^3/gmol), Z_c	190.63, 45.4, 99.418, 0.290
3)	Acentric factor; dipole moment	$\omega = 0.01$, $\mu = 0.00$ D
4)	T_{tp}(K), T_b (K)	90.6, 111.7
5)	At 109.16 K, ρ_1 (g/cm^3)	0.415

6) At 298.16 K

	Cp(1)	Cp°	S°	ΔH^v	$\Delta H_f°$	$\Delta G_f°$
a)	(105.80)	8.54	44.52	19.55	-17.89	-12.15
		(cals/gmol, K)			(kcal/gmol)	
b)	(442.89)	35.74	186.36	81,836	-74,888	-50,860
		(kJ/kgmol, K)			(kJ/kgmol)	

Equations

1) Liquid volume, $V_1 = 5\ (5.7 + 3T_r)$, (cm^3/gmol)

2) Liquid density, $\ln \rho_1 = 1.05536 + 1.24445\ [1 + (1 - T/0.19058E3)^{0.277}]$, ($kgmol/m^3$)

3) Vapor pressure: $\ln P\ (torr) = 15.599 - 968.132/(T - 3.72)$

$\ln P\ (atm) = 8.7119 - 880.601/T - 10430.6/T^2$

4) Mole $Cp°/R = 2.06518 + 7.61373E{-3}\ T - 8.78641E{-7}\ T^2$

5) Mole $Cp(1) = 26.6835 + 0.265361\ T$, (kJ/kgmol, K)

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

7) Surface tension, $\sigma = 0.035684\ (1 - T_r)^{1.092}$, (N/m)

8) Viscosity, vs: $\log vs\ (cp) = 114.14\ (1/T - 1/57.6)$

A8 - 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 — ω = 0.464, μ = 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 $Cp°/R = 5.40946 + 8.73061E{-2}T - 7.24616E{-5}\ T^2 + 2.49691E{-8}\ T^3$

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

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

(8400 operating hours/y)

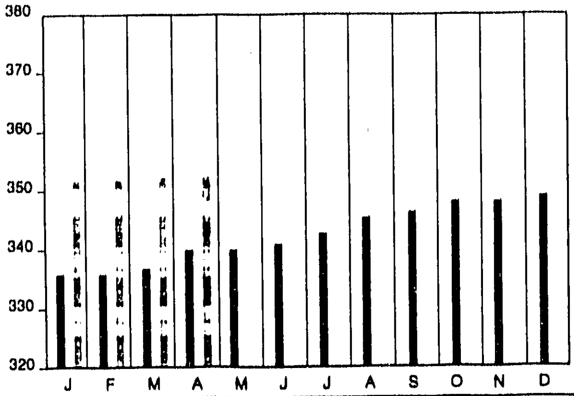
Utility	Amount	Unit Cost	$/h	$/y
1) Natl. gas	2.183E6 Btu/h*	$1.30/E6 Btu	2.838	2.384E4
2) CW	2.429E5 lbm/h 2.916E4 gal/h	$0.10/1000 gal	2.916	2.449E4
3) Steam, 150 psia	3.573E3 lbm/h	$1.58/1000 lbm	5.645	4.742E4
500 psia	5.01E3 lbm/h	$2.20/1000 lbm	11.02	9.257E4
4) Electrical power,** a) pumps	7.650E3 kJ/h	$0.041/kWh	0.8713	7.319E3
b) lights, instru., comp.	7.650E3 kJ/h	$0.041/kWh	0.8713	7.319E3
			$24.16/h	$0.2029E6/y

* 1 Btu = 1.055 kJ

** plant generated

1988 1989

CHEMICAL ENGINEERNG PLANT COST INDEX

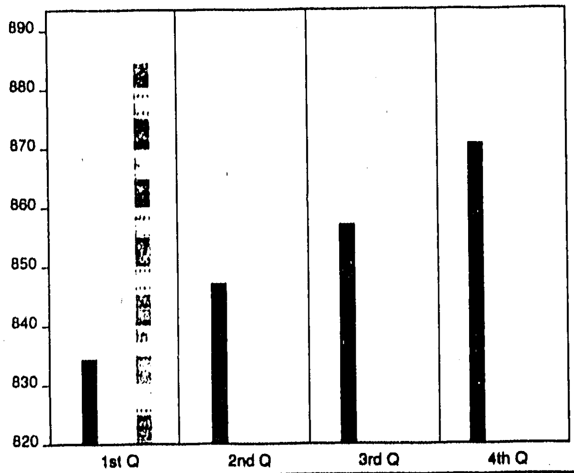


(1957-59 = 100)	Apr.'89 Prelim.	Mar.'89 Final	Apr.'88 Final
CE INDEX	**354.2**	**354.2**	**340.1**
Equipment	**391.0**	**390.7**	**369.4**
Heat exchangers & tanks	372.6	372.5	352.8
Process machinery	360.4	360.5	342.6
Pipe, valves & fittings	463.6	463.5	427.5
Process instruments	351.9	353.0	338.9
Pumps & 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

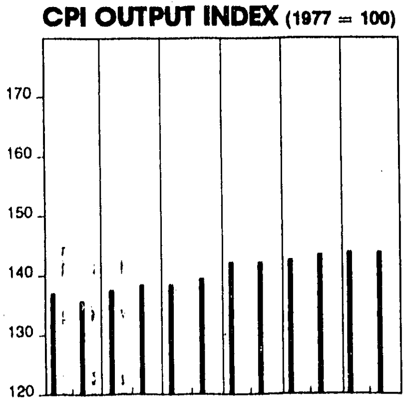
Annual Index

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

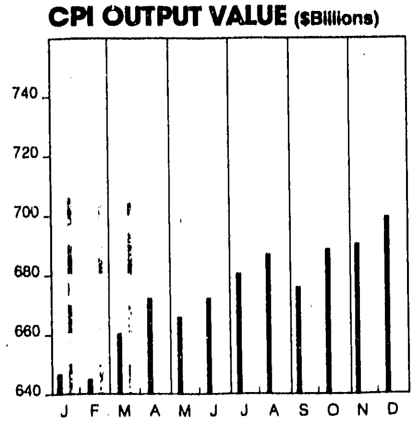
CURRENT BUSINESS INDICATORS

	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

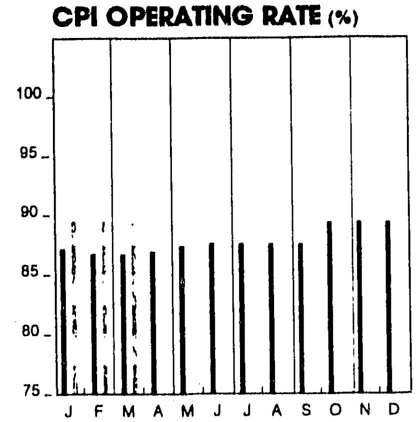
CPI OUTPUT INDEX (1977 = 100)



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
G, L	gas mole flow rate, liquid mole flow rate
ΔG_f^o	Gibbs free energy of formation
G_{max}	maximum gas flow rate
ΔH_f^o, ΔH^v	enthalpy of formation, enthalpy of vaporization
I_c, Inc, PI	cost index, income, plant income
LK, HK	light key, heavy key components
M_i	molecular weight
MC	material of construction
MW	methanol-water fractionator
P, P_c	pressure, critical pressure
PCX, PF	phenol-cresol-xylenol, primary fractionators
POC, T_{op}	plant operating cost, total operating cost
Q	heat transfer rate
Re	Reynolds number
REAC, R_m	reactor, raw material cost
S^o	perfect gas state entropy
S_f, 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
V_{max}	maximum vapor velocity
X_i, Y_i	liquid and vapor mole fractions
Z, Z_c	compressibility factor, critical Z

lower case

h	individual heat transfer coefficient
vs	liquid viscosity

<u>Greek</u>

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

Document Control Page	**1. SERI Report No.** SERI/TP-253-4276	**2. NTIS Accession No.** DE91002141	**3. Recipient's Accession No.**

4. Title and Subtitle Synthesis of Cresols and Xylenols from Phenol and Methanol	**5. Publication Date** April 1992 **6.**
7. Author(s) H. W. Prengle, Jr., X. van Tran, K. Moinzadeh, F. A. Bricout, S. Alam	**8. Performing Organization Rept. No.**
9. Performing Organization Name and Address University of Houston 4800 Calhoun Houston, Texas 77004	**10. Project/Task/Work Unit No.** **11. Contract (C) or Grant (G) No.** (C) XX-7-07028-1 (G)
12. Sponsoring Organization Name and Address Solar Energy Research Institute 1617 Cole Boulevard Golden, Colorado 80401-3393	**13. Type of Report & Period Covered** Technical Report **14.**

15. Supplementary Notes
SERI Technical Monitor: R. Gerald Nix, (303)231-1757

16. Abstract (Limit: 200 words)
This report is the first of two reports that concern the manufacture of the same chemicals using two processes--a conventional catalytic process and a solar photothermal catalytic process--to determine the relative process economics. The results of a process study and evaluation for the synthesis of cresols and xylenols using a conventional catalytic process are presented in this report. (The solar photothermal catalytic process is evaluated in the second report, Synthesis of Cresols and Xylenols from Benzene and Methanol.) The process was a vapor-phase methylation of phenol using a high mole ratio of methanol over a solid acidic catalyst. An arbitrary base case plant size (fresh feed) of about 7 million kg/y (15.3 million lbm/y) was chosen and then escalated to a breakeven size. It was concluded that if a chemical company could obtain a fair share of the market, an estimated profitable operation would result for a plant size greater than 12.80 E6 kg/y of fresh feed.

17. Document Analysis
a. Descriptors
Catalytic process; cresols; xylenols; synthesis; phenol; methanol

b. Identifiers/Open-Ended Terms

c. UC Categories
248

18. Availability Statement National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, VA 22161	**19. No. of Pages** 42 **20. Price** AO3

Form No. 0069E (6-30-87)

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DATE FILMED

7/13/92