NEW PHOSGENE-FREE ROUTE TO POLYCARBONATES

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Senior Design Report

April 9, 2013

University of Pennsylvania

Department of Chemical and Biomolecular Engineering

Faculty Advisor: Prof. Leonard Fabiano, Dr. Raymond Gorte

Recommended by: Mr. Bruce Vrana, DuPont Engineering Technology

April 2, 2013

Department of Chemical and Biomolecular Engineering
School of Engineering and Applied Science
University of Pennsylvania
220 South 33rd Street
Philadelphia, PA 19104

Dear Mr. Fabiano, Dr. Gorte, and Mr. Vrana,

The following is our proposed process design of a phosgene-free route to diphenyl carbonate (DPC) in response to the "New Phosgene-Free Route to Polycarbonates" problem statement posed by Mr. Bruce Vrana of DuPont Engineering Technology. Our design features a new phosgene-free route to produce diphenyl carbonate via the oxidative carbonylation of phenol. After evaluating several design alternatives, we believe that our design is both technologically feasible and economically viable.

Enclosed in this report is our design to produce 100 million pounds of diphenyl carbonate per year, as specified in the problem statement. This report includes details of the proposed process design, all required equipment, expected utility requirements, and an economic analysis. An ASPEN flow sheet and simulation summary are included as well. This report also includes the assumptions that were made in designing this process as well as other considerations that we believe must be taken into account before this process can be implemented. Based upon these measures, we recommend that the project proceeds as designed.

We would like to thank Professor Leonard Fabiano, Dr. Raymond Gorte, Mr. Bruce Vrana, Mr. Richard Bockrath, Mr. John Wismer, Mr. Steven Tieri, and Mr. Adam Brostow for all of their guidance and assistance during this project. Please contact the design team with any questions regarding this report.

Sincerely,

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Federico Castro Imran MacMillan

_____ _____

Abigail Jablansky Heui Beom Lee

Table of Contents

Abstract

Abstract

A process to produce 100 million pounds per year of diphenyl carbonate (DPC) based on the phosgene-free oxidative carbonylation of phenol in US Patent 8,212,066 has been designed. In this reaction, phenol reacts directly with carbon monoxide in the presence of a palladium catalyst, an organic co-catalyst or ligand, a redox catalyst, and a base catalyst. The proposed design features a single-reactor system followed by a separation train that includes a vacuum distillation tower, and it produces only water and carbon monoxide as byproducts. Detailed process and unit descriptions, an in-depth economic analysis, and environmental concerns and other considerations are also included. The net present value of this project was determined to be $51,560,200 with a return on investment of 37.69% and an internal rate of return of 36.1%.

Introduction

Introduction

Diphenyl Carbonate (DPC)

Diphenyl carbonate (DPC), shown in Figure 1, is a common and important intermediate in the production of polycarbonates, which are essential chemicals in many different industries. Polycarbonates are long chains of carbonate oligomer groups that may contain other functional groups. Known for their impact strength, high resistance to heat, and transparency, polycarbonates such as Bisphenol A Polycarbonate, known as BPA-PC or simply BPA, are commonly used to produce plastics used in electrical, construction, automobile, and optical information industries.

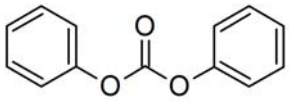
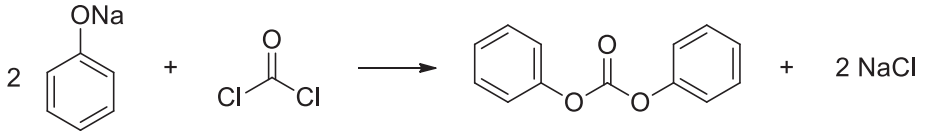


Figure 1: *Molecular structure of DPC*

Traditional Route to DPC

DPC has traditionally been produced via phosgene, a hazardous chemical that is highly toxic to humans and animals, and this report describes a phosgene-free process for producing DPC. While the use of phosgene to produce DPC is profitable and has become the standard practice, it presents significant drawbacks that motivate the development of phosgene-free processes. To produce DPC from phosgene, sodium phenolate is reacted with phosgene to give DPC and sodium chloride, as shown in Reaction 1. This process is hazardous and wasteful, producing large amounts of solid inorganic byproduct.



Rxn. (1)

This first step in this traditional route to DPC, which is described in US Patent Application US2010/0286431, mixes aqueous sodium hydroxide, phenol, and phosgene in a methylene chloride solvent in the presence of an organic amine catalyst. The organic phase is then separated from the aqueous phase, which is discarded as waste water, and the DPC solution is washed with hydrochloric acid and water. Removal of the solvent gives 99.9% pure DPC.

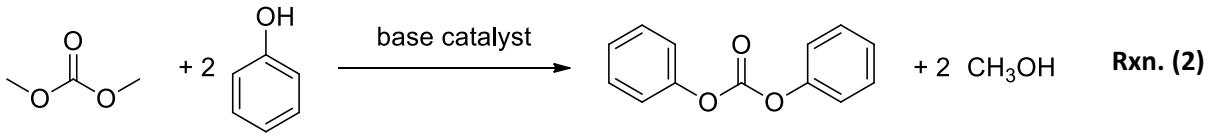
The waste water is freed of solvent residues and catalysts by stripping with steam. After neutralization with hydrochloric acid and treatment with activated carbon, the waste water is fed to an osmotic distillation unit. The concentrated aqueous solution of sodium chloride is then fed to an electrolysis unit, where sodium hydroxide and chlorine is produced. Sodium hydroxide is taken from the cathode side and used directly in the reactor section. Chlorine is taken from the anode side and reacted with carbon monoxide to produce phosgene.

Because of phosgene's significant safety hazards, this process presents substantial costs for proper documentation and approval as well as for proper training and protective equipment. All process equipment that comes in contact with phosgene must be made of corrosion-resistant material, and pumps and other equipment with seals require double seals and a pressurized barrier fluid. Additionally, plants that use phosgene must be built in remote, isolated areas, and special detectors and protective gear and monitors as well as extra safety training are required for all personnel working at these facilities.

Alternative Methods to DPC

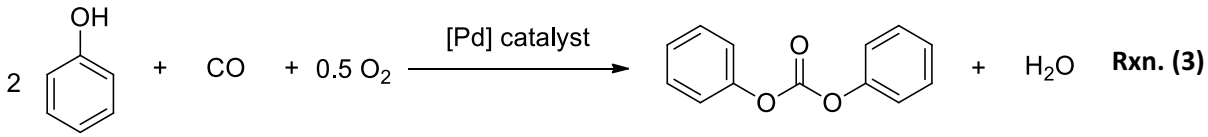
Two phosgene-free methods of DPC production have been developed to alleviate the costs and safety hazards associated with phosgene use while still profitably producing DPC. The first is the transesterification of dimethyl carbonate, in which dimethyl carbonate is reacted with two equivalents of phenol to give DPC and methanol as shown in Reaction 2. Dimethyl carbonate is readily synthesized

from methanol and carbon monoxide through a process called oxidative carbonylation (Serini, "Polycarbonates"). While this mechanism presents a much safer alternative to the phosgene method, this reaction suffers from low conversion, since phenol is five times more acidic than methanol is.

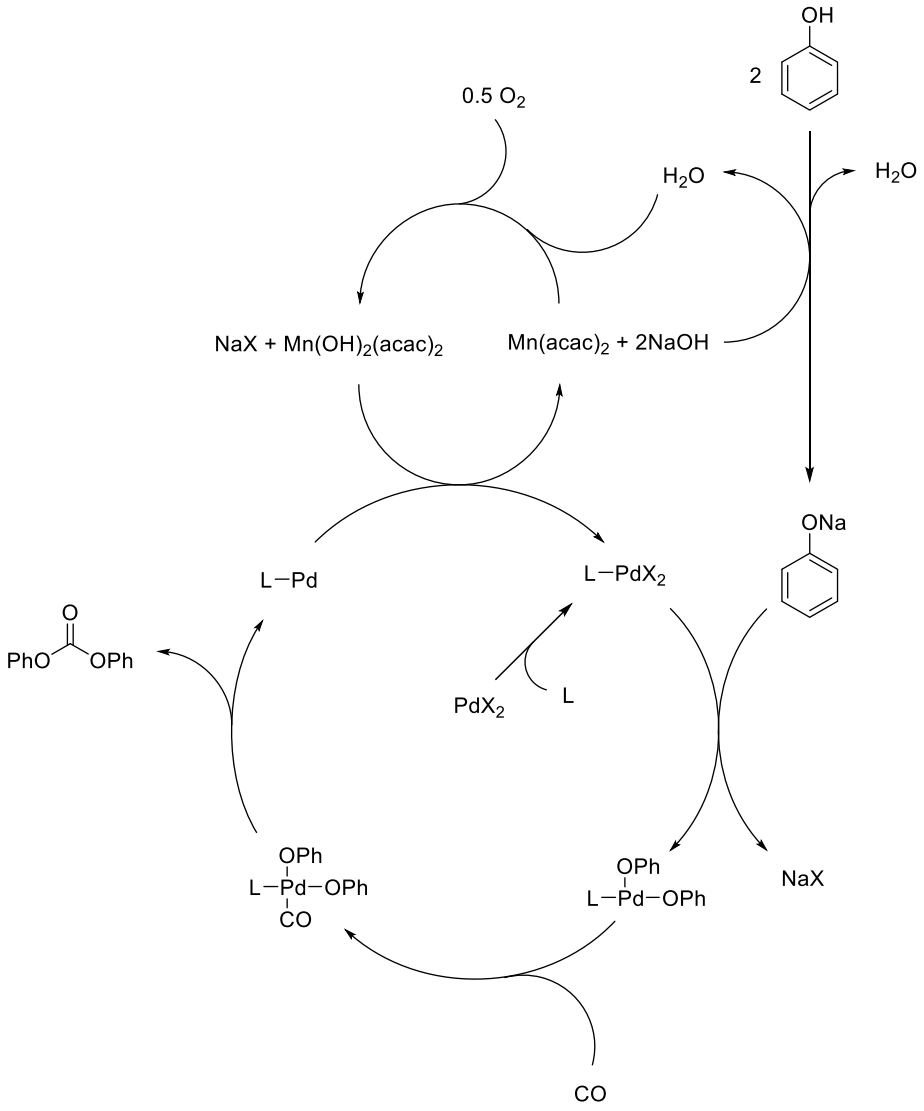


Rxn. (2)

The second phosgene-free route to DPC is the oxidative carbonylation of phenol and is described in this report. This novel synthesis of DPC, described in US Patent 8,212,066, involves the palladium-catalyzed oxidative carbonylation of phenol in which phenol is reacted directly with carbon monoxide in the presence of a palladium catalyst, an organic co-catalyst (ligand), a redox catalyst, and a base catalyst. This is a simple process that uses cheap, non-toxic reagents and whose only byproduct is water. The overall reaction is given by Reaction 3:



Rxn. (3)



Mechanism 1: Mechanism for the palladium-catalyzed oxidative carbonylation of phenol to DPC.

As shown in Mechanism 1, oxidative carbonylation is the process by which carbon monoxide is inserted into an organic substrate under the action of a metal catalyst. The catalyst for the above-proposed mechanism consists of a Pd(II) species coordinated to an organic co-catalyst (ligand, represented by L). In the first step, phenol is deprotonated by action of the base NaOH, generating phenoxide ions which undergo transmetallation with the Pd catalyst. After carbon monoxide is

coordinated to the metal, the coordinated phenoxide ions then insert into the carbon oxygen triple bond. After reductive elimination, the reduced Pd(0) species and the product DPC is obtained.

The metal reoxidation process has always been a major problem in oxidative carbonylation; and it is known that direct reoxidation with molecular oxygen is possible in the presence of a transition metal catalyst based on copper, manganese, or cobalt. Using molecular oxygen as the terminal oxidant is desirable since the byproduct of the reaction is water. According to the above mechanism, only a sub-stoichiometric amount of sodium hydroxide is necessary. Tetrabutyl ammonium iodide serves as a phase transfer catalyst.

The oxidation of phenols often produces a number of products that are sometimes polymeric and quinonoid in nature. Generally, the oxidation of phenols involves the removal of one hydrogen atom from each phenol molecule and leads exclusively to ortho- and para-linked dimeric and polymeric products, predominantly containing carbon-carbon and, more rarely, carbon-oxygen bonds.

It has been shown in the literature that manganese(III) acetylacetonate could be used as a catalyst for the oxidation of phenol (Musso, 1963). The terminal oxidant used for the catalytic oxidation of phenol is molecular oxygen. Possible side products for the oxidative carbonylation of phenol are summarized in Table I on the following page.

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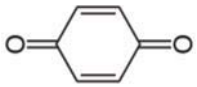
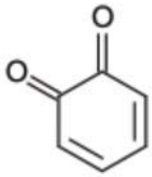
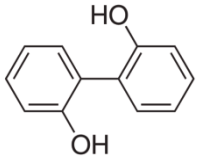
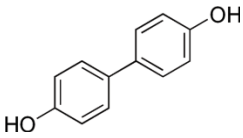
Table I: *Possible byproducts of the oxidative carbonylation of phenol*

Possible Side Product	Molecular Structure	Melting Point	Boiling Point
1,4-benzoquinone		239°F	Sublimes
1,2-benzoquinone		Not available	415.4°F
2,2'-biphenol		228.2°F	599°F
4,4'-biphenol		545°F	Sublimes

The products listed in Table I may not separate from phenol, from diphenyl carbonate, or from the catalysts. A purge stream located at the catalyst recycle stream was designed to prevent the buildup of these possible byproducts. Fortunately, under the reaction conditions specified in the patent where oxygen is the limiting reagent, the selectivity for DPC is greater than 99%, and the formation of byproducts and non-volatile byproducts may be assumed to be minimal. Therefore, water is assumed to be the only significant byproduct in this process.

This report describes a process of producing 100 million pounds of DPC per year using the phosgene-free oxidative carbonylation process based on US Patent 8,212,066 and shown in Mechanism 1. The proposed design avoids the high costs and safety precautions needed when using phosgene, and it considers recycling as much unused material as possible, using non-toxic chemicals, and using as minimal energy as possible in order to promote chemical, environmental, and economic sustainability.

Project Charter

Project Charter

Project Name	New Phosgene-Free Route to Polycarbonates
Project Champions	Federico Castro, Abigail Jablansky, Heui Beom Lee, Imran MacMillan
Project Leader	Mr. Bruce Vrana, DuPont
Specific Goals	More environmentally friendly approach to synthesizing diphenyl carbonate
Project Scope	In-scope: • Manufacture of diphenyl carbonate using oxidative carbonylation • Key starting materials: phenol, carbon monoxide, oxygen • Key Catalysts: Palladium chloride, sodium hydroxide, $Mn(acac)_2$, $[^nBu_4N]I$, 3,6-diaminocarbazole • Achieve a profitable process • Ensure final product DPC is distributable Out-of-scope: • Distribution and shipment of final product • Establishing customers and finalizing sales
Deliverables	Business Opportunity Assessment: • What is the marketability of the 100 million pounds a year of DPC production? • What kind of growth is the market expecting in the near future? Technical Feasibility Assessment: • Is it possible to produce 100 million pounds a year of DPC? Manufacturing capability assessment: • Can a facility be built to manufacture 100 MM lb/yr of DPC without insurmountable capital investment?
Timeline	First deliverable production will occur two years after initiating construction

Innovation Map

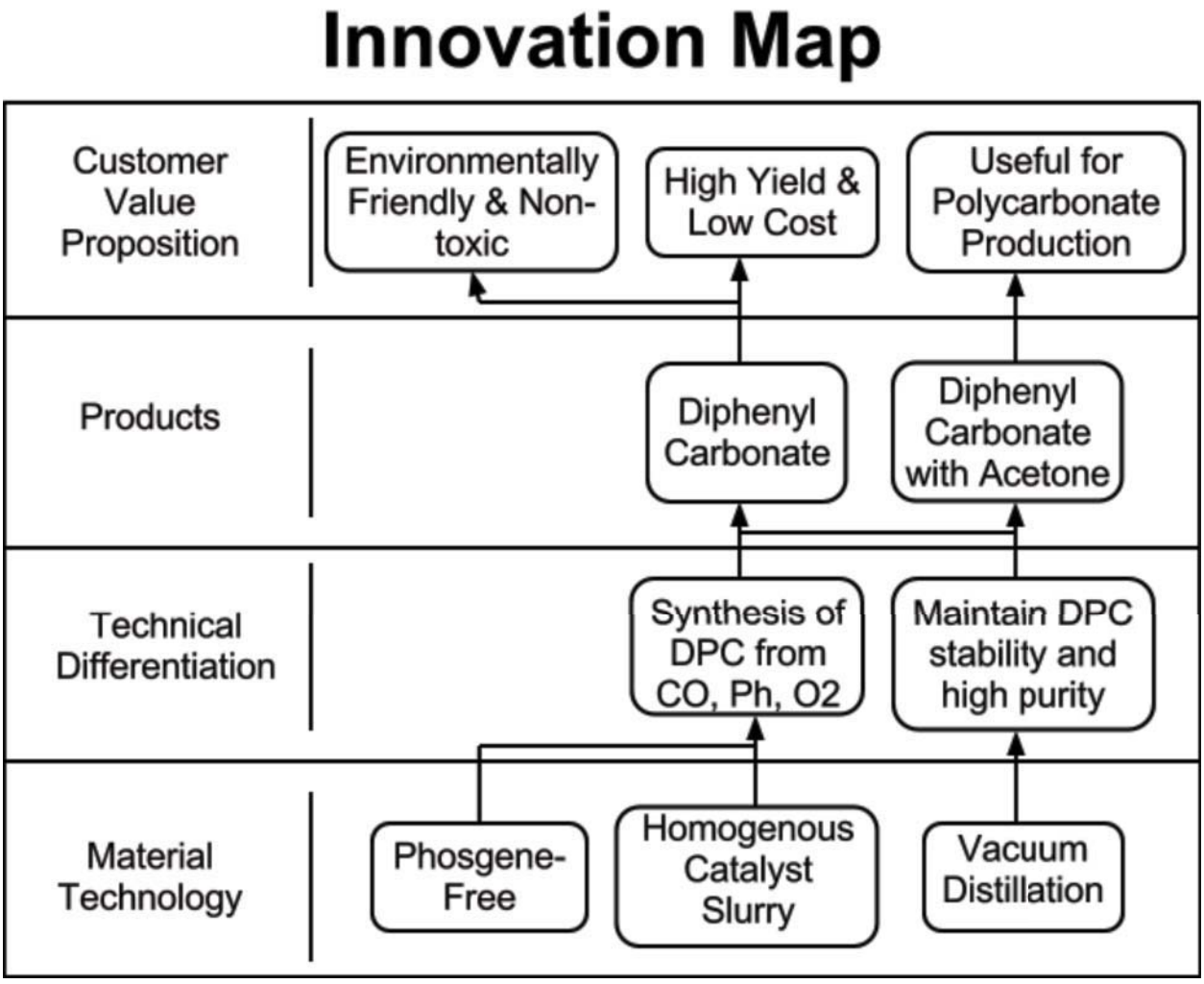


Figure 2: Innovation Map

The innovation map given in Figure 2 presents the technological advantages that the process proposed in this report has over the traditional phosgene method of DPC production. Most notably, the phosgene-free process described here avoids the high costs associated with proper approval and documentation and with specialized equipment, protective gear and monitors, and safety training. Additionally, the homogeneous catalyst slurry used in this phosgene-free process replaces the methylene chloride solvent and acidic solvent removal process and decreases the number of blocks as well as the cost associated with more raw materials and more waste. The waste from the phosgene-free process consists of just water and carbon monoxide, while the waste from the traditional phosgene process includes sodium chloride and phosgene.

In both processes, the reactions occur at low temperatures and with very high selectivity for DPC. Although the phosgene-free process requires a higher pressure and a longer residence time, the process presented in this report achieves the same goal as the traditional phosgene process without the added costs of safety, raw materials, and special equipment that are necessary when working with phosgene. Furthermore, this phosgene-free process presents significantly lower health and environmental risks to those living and working in or near plants that use phosgene.

Concept Stage: Market and Competitive Analyses

Market and Competitive Analyses

Diphenyl Carbonate (DPC)

Commodity-scale production of industrial chemicals depends heavily on current and anticipated market conditions due to high capital investment costs and long-term returns. As a high-volume producer of DPC representing 5-10% of global production over the next five years, we will be a significant entrant into the marketplace. The global production of DPC in 2002 was reported as 254,000 tonnes, or 559,974,000 pounds ("Global Plastic Product and Packaging Manufacturing industry Outlook", IBISWorld). DPC production was split among dozens of producers operating out of Western Europe, Japan and the Far East; with the majority of DPC production occurring outside of North America, there is a lot of potential to capture local market share with domestically produced DPC ("Diphenyl Carbonate", OECD SIDS). The recent upward trend in domestic industrial investment will provide a good climate for the large investments necessary to finance a high capital cost facility such as the one described in this report. The diversity of suppliers—over 100,000—also decreases the competitive barrier to entry because no single entity has captured a majority of market share ("Products and Markets", IBISWorld). Another advantage of opening a DPC production plant in the Gulf Coast is easy access to advanced distribution networks thanks to heavily developed infrastructure, which makes it easy to ship DPC to various buyers.

The largest use of DPC comes from the synthesis of thermoplastics and polycarbonates (PCs), such as the commonly used Bisphenol-A (BPA), and it is assumed that the market conditions driving DPC demand and PC demand are the same. The primary uses of DPC include packaging materials, consumer goods, automotive goods, aviation instrumentation, and construction services and require at least 98% pure DPC. However, global demand tied to consumer products is decreasing because of two main factors: environmental concerns and personal health concerns. Increasing environmental concerns are leading to minimization of package sizing, and improvements in the recycling process are lessening the

global demand for these plastics. The sensitivity of this consumer market is also highlighted by the recently released research findings exposing BPA as a cancer promoting agent (Braun, 2009; Li, 2009; Lang, 2008). This has far-reaching applications for the future of BPA production, as the search for alternatives has rapidly accelerated and BPA is being phased out as a whole.

However, one important reason that plastics are gaining market share over substitute goods, such as glass and aluminum, is that current technological innovation is leading to an expanded range of products for PCs. This implies that the potential market for DPC will be strong.

Figure 3 and Table II show a market projection of the global plastic product and packaging industry which shows that, despite recent concerns, the plastics industry will be able to grow due to technological innovation that decreases manufacturing costs and accounts for plastic preference over substitute goods.

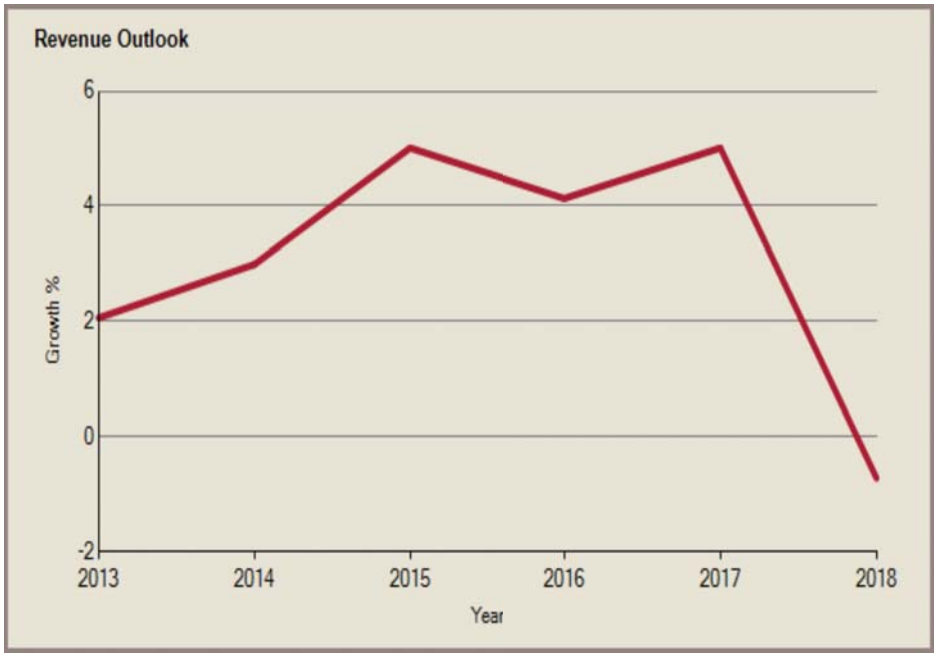


Figure 3: *Plastics projected revenue growth over the next five years ("Products and Markets", IBISWorld)*

Table II: *Plastics projected revenue growth over the next five years ("Products and Markets", IBISWorld)*

Revenue Outlook		
Year	**Revenue $ (millions)**	**Growth %**
2013	795,902.40	2.1
2014	819,722.50	3
2015	860,856.20	5
2016	896,427.00	4.1
2017	941,409.80	5

Preliminary Process Synthesis

Preliminary Process Synthesis

The production of diphenyl carbonate (DPC) presented in this report is based on the oxidative carbonylation of phenol, as described in US Patent 8,212,066, filed by China Petrochemical Devlopment Corporation in 2012, which is given in the Appendix of this report. The reaction is promoted by base (sodium hydroxide) and catalyzed by palladium chloride ($PdCl_2$), an organic ligand (carbazole or a carbazole derivative), a phase transfer catalyst (tetra-n-butylammonium chloride), and an inorganic redox catalyst (manganese diacetylacetonate).

Since limited information is given regarding this phosgene-free route to DPC, the design for this process was based largely on US Patent 8,212,066. The block diagram of the proposed design is shown in Figure 4 below:

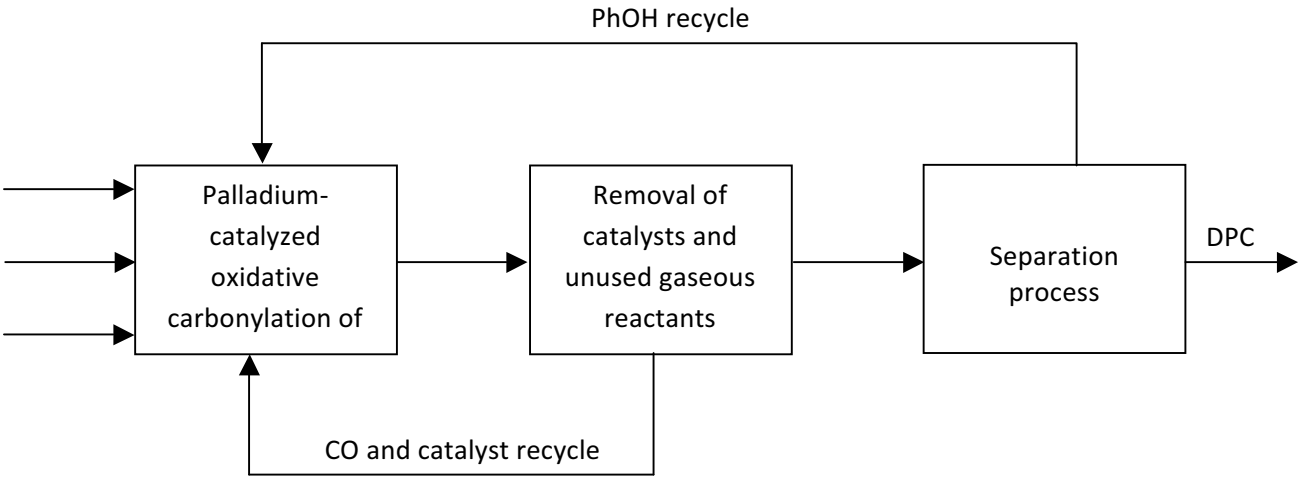


Figure 4: *Block flow diagram for the production of DPC*

Figure 4 shows the three different sections of the DPC production process described in this report. In the first section, a continuously stirred tank reactor (CSTR) is fed phenol, oxygen, carbon monoxide, and a catalyst mixture consisting of palladium chloride, sodium hydroxide, $Mn(acac)_2$, $[^nBu_4N]I$, and 3,6-diaminocarbazole. All steps of the reaction occur inside the reactor, including the

oxidative carbonylation of phenol, the regeneration of the catalysts, and the production of water as a byproduct. The reaction is quite exothermic, and the catalysts remain in a homogeneous state throughout the reaction.

The reactor effluent, still at a high temperature and pressure, passes through a series of two flash vessels, which remove the gases and catalysts from the liquid products and unused reactants. The first flash vessel separates oxygen, unreacted carbon monoxide, and a small amount of water from the DPC, unreacted phenol, and catalysts, and most of the carbon monoxide is recycled back to the reactor; the rest is purged. The second flash vessel operates under a vacuum system and separates the catalyst mixture from the DPC, unreacted phenol, and water. Most of the catalyst mixture is recycled to the reactor; a small amount is purged along with impurities.

The final stage in the process is the separation train. The DPC, phenol, and water enter the first distillation tower, which also operates under a vacuum. Vacuum conditions are required to attain a 98% pure stream of DPC, the heaviest product, without it decomposing at temperatures occurring under normal pressures. The DPC stream is then pumped and condensed to be delivered under manageable conditions. The water and phenol stream that leaves the top of the first distillation tower is compressed, flashed, and distilled at atmospheric pressure in order to recycle as much phenol and as little water to the reactor as possible.

This process was designed to produce a target product specification of 100 million pounds per year of DPC under an operating schedule of 8620 hours per year. The following section provides the full process flow diagram and material balances for this process.

Process Flow Diagram and Material Balances

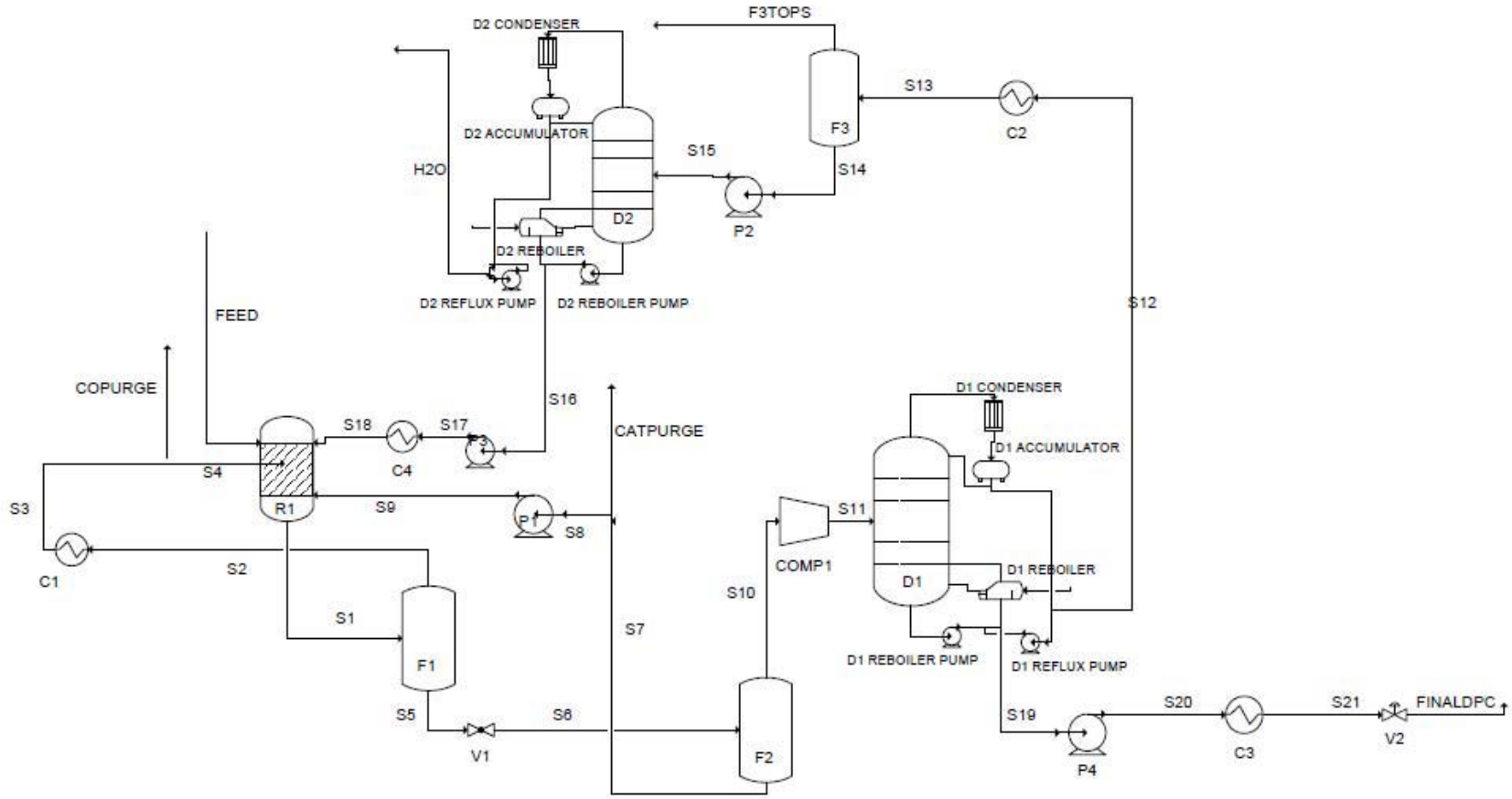


Figure 5: *Process flowsheet*

Table III: *Stream information for entire process*

	FEED	S1	S2	S3	COPURGE	S4	S5	S6	S7
Temperature F	176.00	176.00	176.00	77.00	77.00	77.00	176.00	134.60	248.00
Pressure psia	145.04	145.04	145.04	145.04	145.04	145.04	145.04	0.15	0.15
Vapor Frac	0.52	0.30	1.00	1.00	1.00	1.00	0.00	0.10	0.00
Mole Flow lbmol/hr	257.11	1869.46	552.98	552.98	27.65	525.33	1316.49	1316.49	1.36
Mass Flow lb/hr	15400.14	140950.18	15530.50	15530.50	776.53	14753.97	125419.68	125419.68	230.30
Enthalpy MMBtu/hr	-12.48	-119.16	-26.02	-26.44	-1.32	-25.12	-93.14	-93.14	-0.09
Mass Flow lb/hr									
PHENOL	11502.46	110989.83	91.65	91.65	4.58	87.07	110898.17	110898.17	38.00
WATER	0.00	1114.73	41.43	41.43	2.07	39.36	1073.31	1073.31	0.00
DPC	0.00	12877.22	0.00	0.00	0.00	0.00	12877.22	12877.22	127.66
CO	2944.68	15903.76	15397.41	15397.41	769.87	14627.54	506.34	506.34	0.00
O2	952.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.65	64.64	0.00	0.00	0.00	0.00	64.64	64.64	64.64
Mass Frac									
PHENOL	0.75	0.79	0.01	0.01	0.01	0.01	0.88	0.88	0.17
WATER	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00
DPC	0.00	0.09	0.00	0.00	0.00	0.00	0.10	0.10	0.55
CO	0.19	0.11	0.99	0.99	0.99	0.99	0.00	0.00	0.00
O2	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28

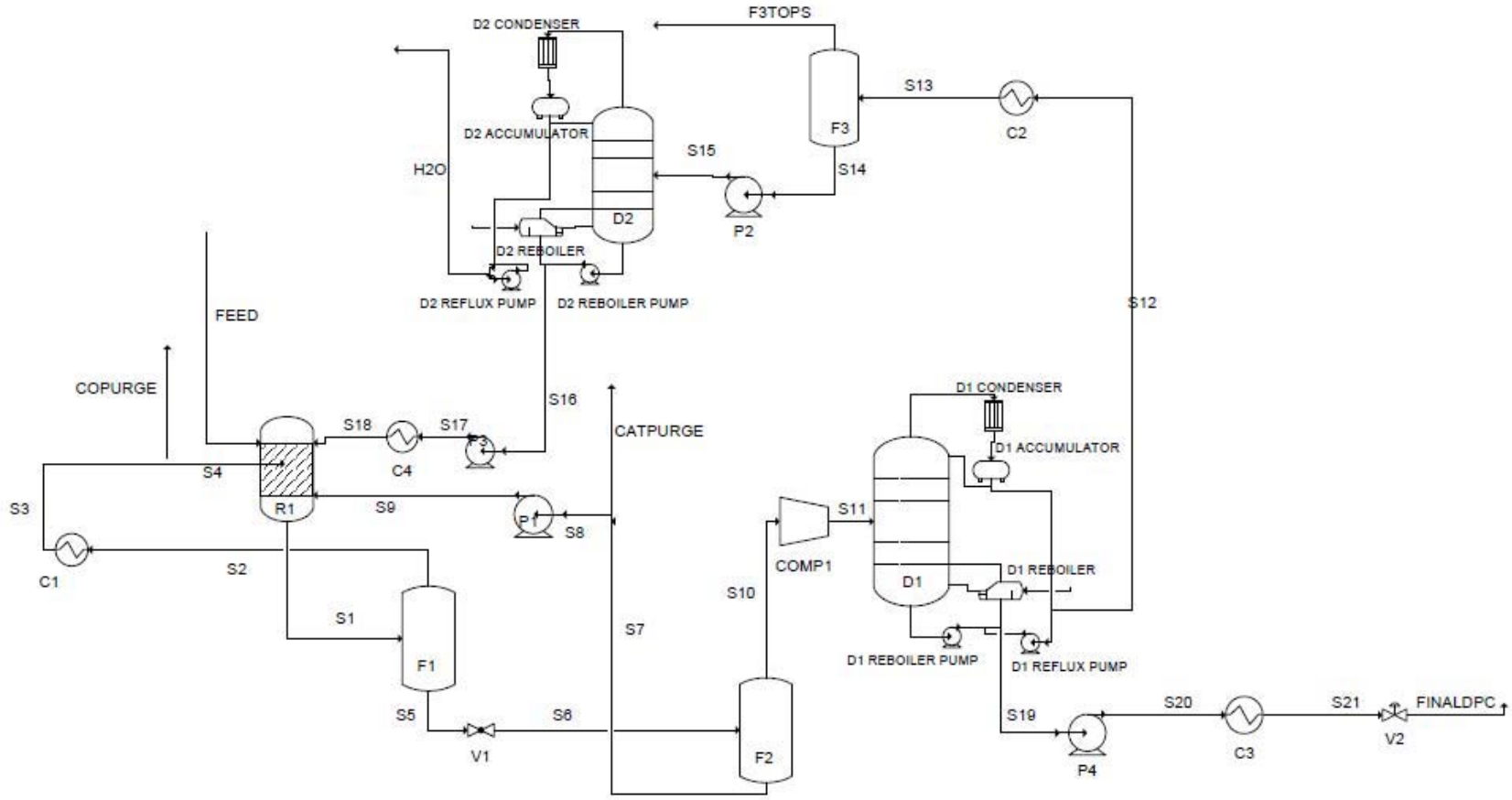


Figure 5: *Process Flowsheet*

***Table III (continued)**: Stream information for entire process*

	CATPURGE	S8	S9	S10	S11	S12	S13	F3TOPS	S14
Temperature F	248.00	248.00	252.80	248.00	387.90	190.90	77.00	77.00	77.00
Pressure psia	0.15	0.15	203.05	0.15	1.45	0.48	0.48	0.48	0.48
Vapor Frac	0.00	0.00	0.00	1.00	1.00	1.00	0.02	1.00	0.00
Mole Flow lbmol/hr	0.01	1.35	1.35	1315.12	1315.12	1252.94	1252.94	19.71	1233.23
Mass Flow lb/hr	2.30	227.99	227.99	125189.39	125189.39	112189.63	112189.63	559.38	111630.25
Enthalpy MMBtu/hr	0.00	-0.09	-0.09	-59.68	-53.35	-52.03	-85.99	-1.02	-84.98
Mass Flow lb/hr									
PHENOL	0.38	37.62	37.62	110860.17	110860.17	110609.98	110609.98	30.57	110579.42
WATER	0.00	0.00	0.00	1073.31	1073.31	1073.31	1073.31	25.75	1047.55
DPC	1.28	126.38	126.38	12749.56	12749.56	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	506.34	506.34	506.34	506.34	503.07	3.28
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.65	63.99	63.99	0.00	0.00	0.00	0.00	0.00	0.00
Mass Frac									
PHENOL	0.17	0.17	0.17	0.89	0.89	0.99	0.99	0.06	0.99
WATER	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.05	0.01
DPC	0.55	0.55	0.55	0.10	0.10	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.90	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.00

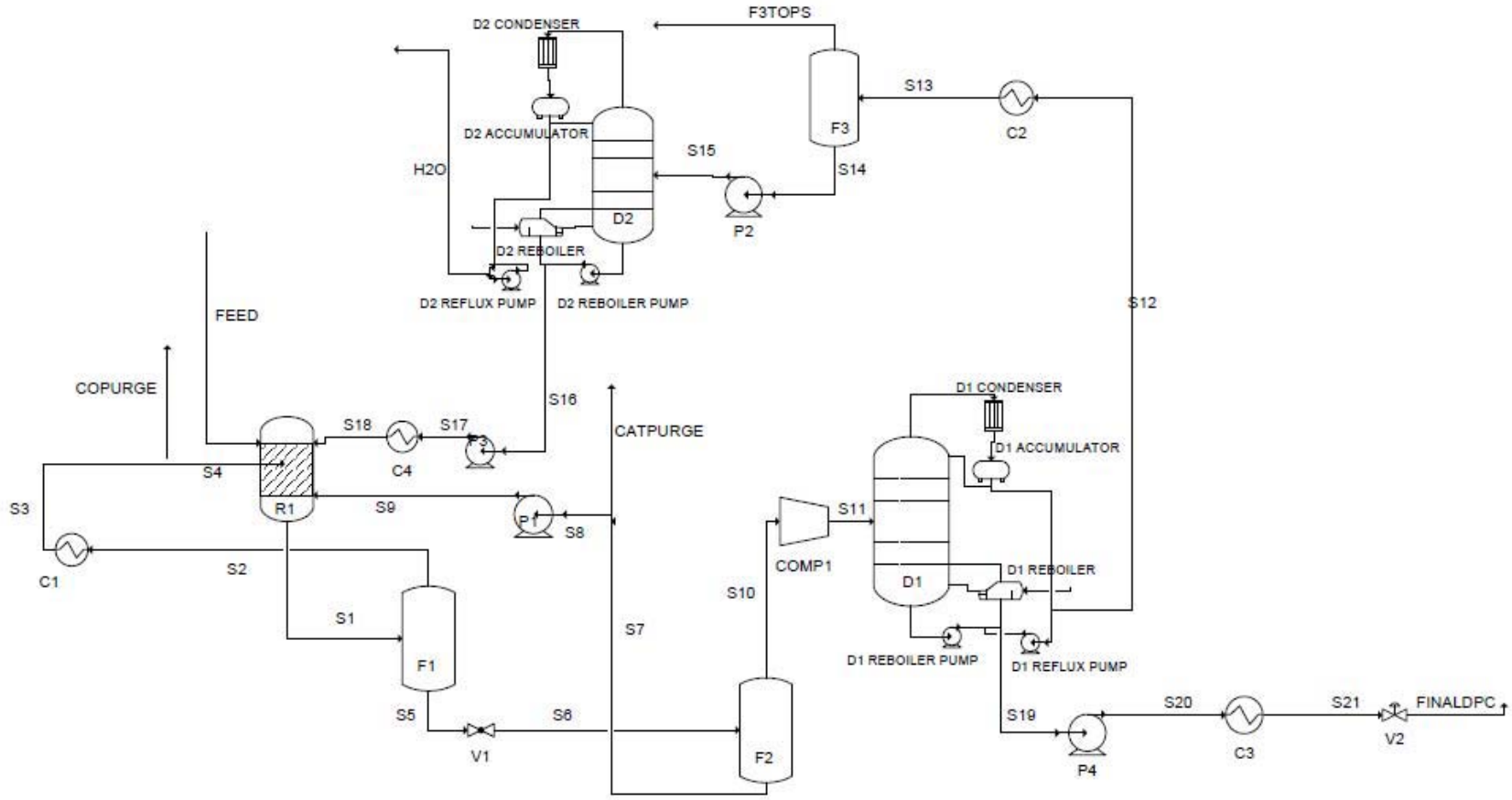


Figure 5: *Process Flowsheet*

***Table III (continued)**: Stream information for entire process*

	S15	H2O	S16	S17	S18	S19	S20	FINALDPC
Temperature F	77.20	211.40	379.70	380.70	194.00	401.40	401.70	212.00
Pressure psia	20.31	14.50	19.85	145.04	145.04	1.01	19.50	14.50
Vapor Frac	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow lbmol/hr	1233.23	58.22	1175.01	1175.01	1175.01	62.18	62.18	62.18
Mass Flow lb/hr	111630.25	1059.24	110571.01	110571.01	110571.01	12999.76	12999.76	12999.76
Enthalpy MMBtu/hr	-84.97	-5.98	-60.70	-60.63	-71.89	-10.79	-10.79	-11.88
Mass Flow lb/hr								
PHENOL	110579.42	11.45	110567.97	110567.97	110567.97	250.19	250.19	250.19
WATER	1047.55	1044.51	3.04	3.04	3.04	0.00	0.00	0.00
DPC	0.00	0.00	0.00	0.00	0.00	12749.56	12749.56	12749.56
CO	3.28	3.28	0.00	0.00	0.00	0.00	0.00	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mass Frac								
PHENOL	0.99	0.01	1.00	1.00	1.00	0.02	0.02	0.02
WATER	0.01	0.99	0.00	0.00	0.00	0.00	0.00	0.00
DPC	0.00	0.00	0.00	0.00	0.00	0.98	0.98	0.98
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PALLA-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

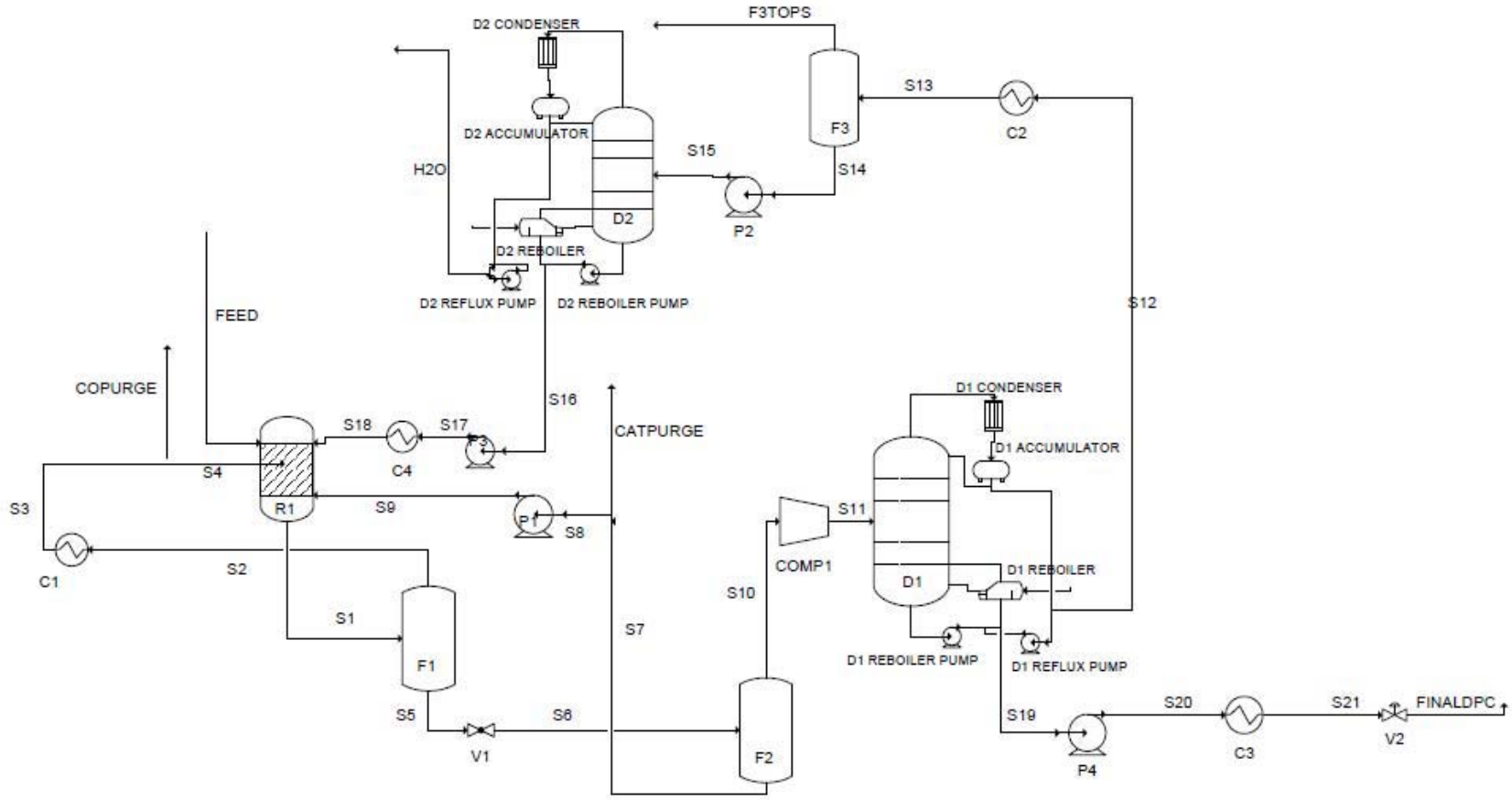


Figure 5: *Process Flowsheet*

Table IV: *Stream information for reactor block*

	IN				OUT
	FEED	**S4**	**S9**	**S18**	**S1**
Temperature F	176.00	77.00	252.80	194.00	176.00
Pressure psia	145.04	145.04	203.05	145.04	145.04
Vapor Frac	0.52	1.00	0.00	0.00	0.30
Mole Flow lbmol/hr	257.11	525.33	1.35	1175.01	1869.46
Mass Flow lb/hr	15400.14	14753.97	227.99	110571.01	140950.18
Enthalpy MMBtu/hr	-12.48	-25.12	-0.09	-71.89	-119.16
Mass Flow lb/hr					
PHENOL	11502.46	87.07	37.62	110567.97	110989.83
WATER	0.00	39.36	0.00	3.04	1114.73
DPC	0.00	0.00	126.38	0.00	12877.22
CO	2944.68	14627.54	0.00	0.00	15903.76
O2	952.36	0.00	0.00	0.00	0.00
PALLA-01	0.65	0.00	63.99	0.00	64.64
Mass Frac					
PHENOL	0.75	0.01	0.17	1.00	0.79
WATER	0.00	0.00	0.00	0.00	0.01
DPC	0.00	0.00	0.55	0.00	0.09
CO	0.19	0.99	0.00	0.00	0.11
O2	0.06	0.00	0.00	0.00	0.00
PALLA-01	0.00	0.00	0.28	0.00	0.00

Process Material Balance

Table V: *Process Material Balance*

INLET STREAM	MASS FLOW, LB/HR	OUTLET STREAMS	MASS FLOW, LB/HR
FEED	15400.14	COPURGE	776.53
		CATPURGE	2.30
		F3TOPS	559.38
		H2O	1059.24
		FINALDPC	12999.76
TOTAL	15400.14	TOTAL	15397.20

As seen in Table V, the law of mass conservation is observed in this process. The inlet stream (FEED) has a flowrate of 15,400.14 pounds per hour, and the outlet streams (COPURGE, CATPURGE, F3TOPS, H2O, AND FINALDPC) have a combined flowrate of 15,397.20 pounds per hour, which is very close to the inlet flowrate.

Process Description

Overall Process Description

Reactor Block

In the first part of the process, shown in Figure 6, phenol and the catalysts are mixed together and fed continuously to the reactor through stream S-1. Carbon monoxide and oxygen are mixed together and fed continuously to the reactor through stream S-2. The pressure and the temperature of the reactor are then adjusted to the conditions required for the oxidative carbonylation of phenol, 10 bar (145 psi) and 80^{o}C (176^{o}F), so as to continually produce as much DPC as possible. The flow rate of the product stream S-3 and the size of the reactor are calibrated such that the mean residence time inside the reactor is 60 minutes.

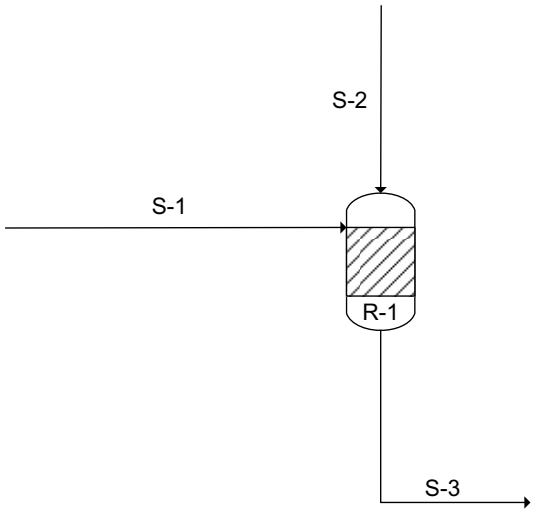


Figure 6: *The reactor system designed in the preliminary process synthesis*

For the synthesis of the separation train, several alternatives have been considered: (i) removal of water through use of a hygroscopic solid desiccant and thermal regeneration thereof after filtration, (ii) recovery of the catalyst through use of multiple liquid-liquid extraction units and subsequent removal of solvent by distillation, and (iii) recovery of the catalyst through flash distillation of the reaction mixture and subsequent purification of the product through vacuum distillation. The third alternative

was deemed to offer the highest recovery of the catalyst while minimizing material and energy costs for the purification of the product. Previous designs featuring the first and second options were considered and are presented in the Appendix, but a distillation-intensive process was deemed the most feasible.

Eliminate differences in composition

Figure 7 illustrates the preliminary separation scheme that was developed to eliminate differences in composition based on the considerations and assumptions above.

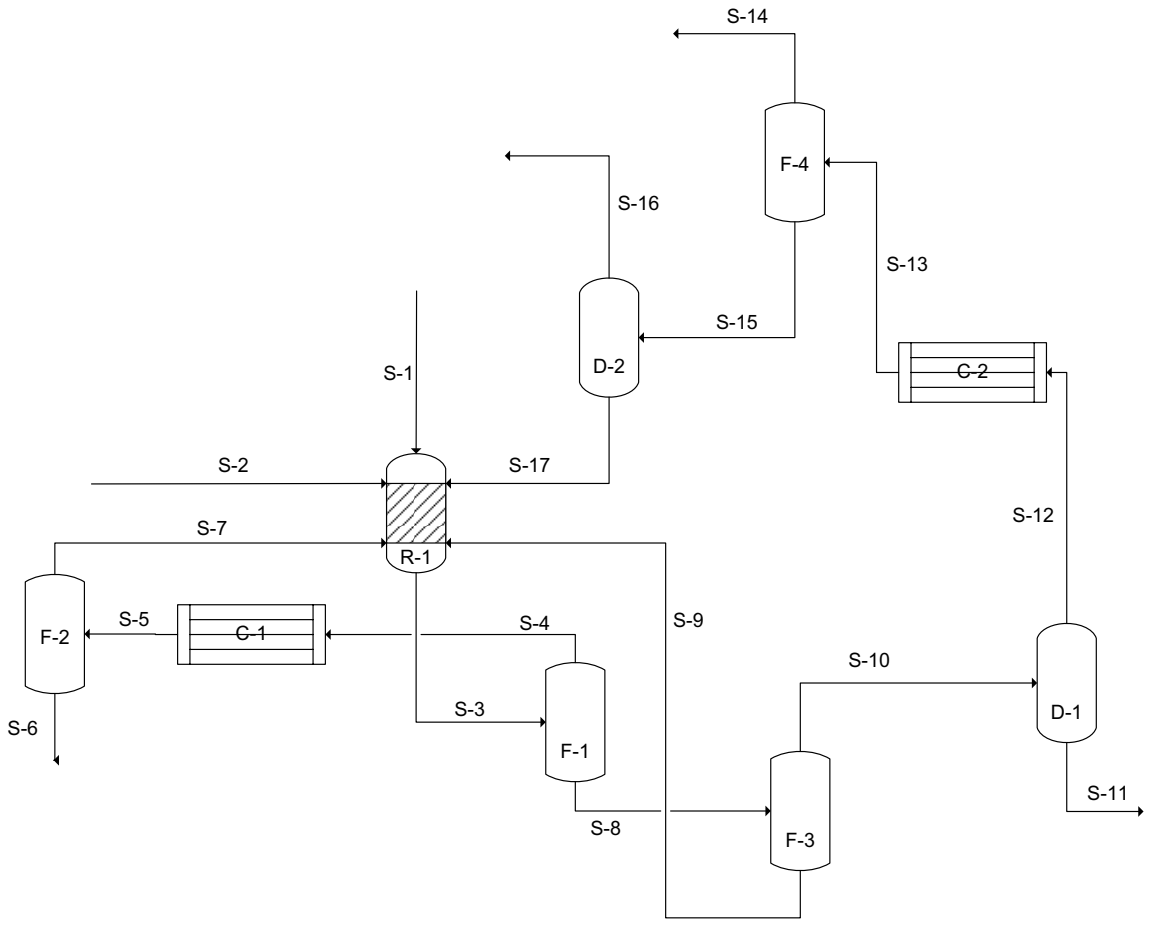


Figure 7: *The reactor block and the preliminary separation scheme for the design*

The outlet of the reactor R-1, the product stream S-3, enters a disengagement vessel F-1 maintained at 10 bar and 80^{o}C. The vapor stream S-4 exiting the disengagement vessel F-1 carries most of the excess unspent carbon monoxide. The vapor stream S-4 then enters a condenser unit C-1 maintained at 10 bar and 25^{o}C to remove small amounts of condensable species such as water and phenol. Stream S-5 then enters a disengagement vessel F-2 where the liquid phase is removed through S-6 and the gas phase is removed through stream S-7. This gas stream carries dried carbon monoxide gas which can be recycled back to the reactor R-1. The liquid stream S-8 from the disengagement vessel F-1 then enters a flash vessel F-3 maintained at 0.01 bar and 120^{o}C. The purpose of this vessel is to separate unused starting materials and the product from the homogeneous catalyst mixture. The homogeneous catalyst mixture is removed through stream S-9 and recycled back to the reactor. The vapor phase leaves the flash vessel F-3 through the stream S-10. Stream S-10 then enters a distillation tower operated at reduced pressures. The purpose of this unit is to separate diphenyl carbonate from excess phenol and water. Nearly pure diphenyl carbonate (>98 wt%) is therefore recovered as the bottoms product through stream S-11. The overhead product contains water, phenol, and a small amount of carbon monoxide which remained in solution. The overhead product is removed through stream S-12. Stream S-12 then enters a condenser unit C-2 operated at 0.03bar and 25^{o}C. After cooling, stream S-13 enters a disengagement vessel F-4. Most of the remaining carbon monoxide exits through stream S-14, and a liquid stream consisting of water and phenol exits through stream S-15. Stream S-15 then enters a distillation tower whose reflux condenser is operated at atmospheric pressure. Nearly pure phenol (>99 wt%) is recovered as the bottoms product through stream S-17 and recycled to the reactor R-1. The overhead product is removed through stream S-16 and discarded.

Eliminate temperature, pressure and phase differences

Figure 8 shows the pumps, compressors, and heat exchangers that complete the process design:

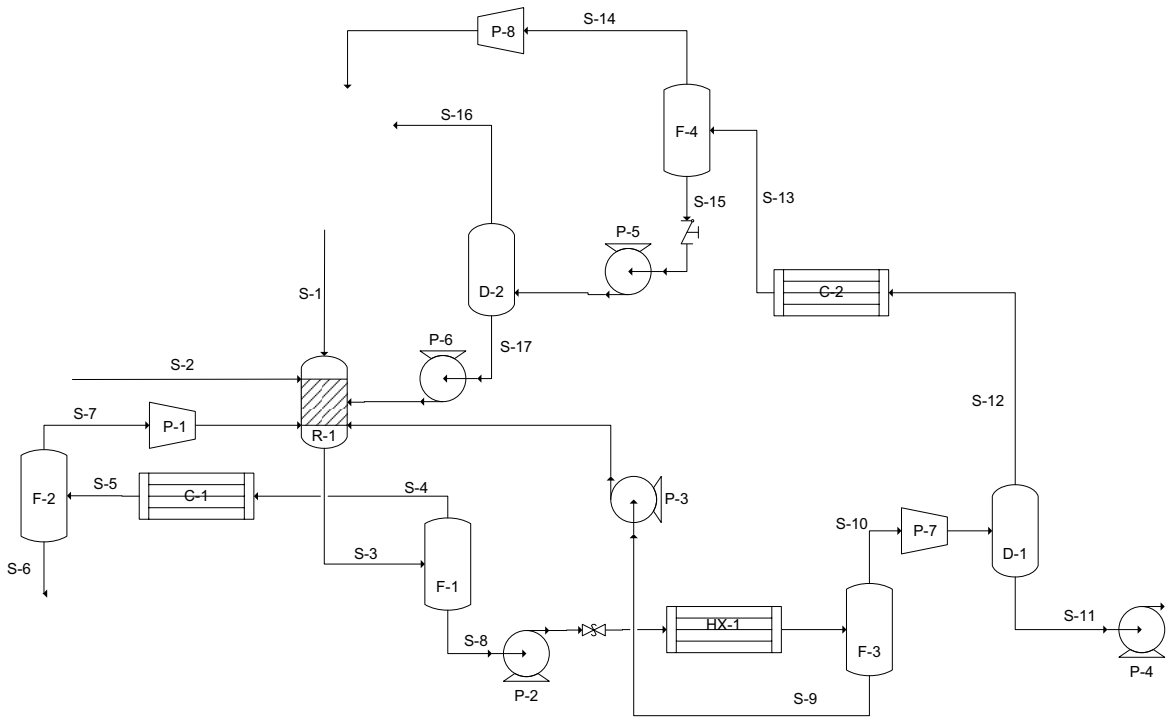


Figure 8: *The reactor, separation scheme, and phase change blocks of the preliminary process design*

Compressor P-1 is used to compensate for the pressure loss due to F-1, C-1, and F-2. After being pumped using pump P-2, stream S-8 passes through a throttling valve that reduces the pressure of the stream down to the pressure required by F-3. The temperature of stream S-8 is adjusted to the flash temperature required by F-3 by using a series of heat exchangers in order to recover heat from utilities such as steam. P-7 represents a vacuum pump that is used to achieve a partial vacuum in the flash vessel F-3. Although not shown in the figure above, both D1 and D2 require the use of reboilers and condensers. P-4 is used to pump the bottoms product of D1. The overhead product of D1 passes through a partial condenser C-2 and then through a disengagement vessel F-4 to remove small amounts

non-condensable carbon monoxide. P-8 represents the vacuum pump that is used to achieve a partial vacuum within D1. The bottoms product S-15 from F-4 passes through a pump P-5. S-15 is then fed to the distillation column D-2 where S-17 is removed as the bottoms product. P-6 is used to pump S-17 which contains nearly pure phenol back to the reactor thus reducing the cost of phenol purchase.

ASPEN Process Flowsheet

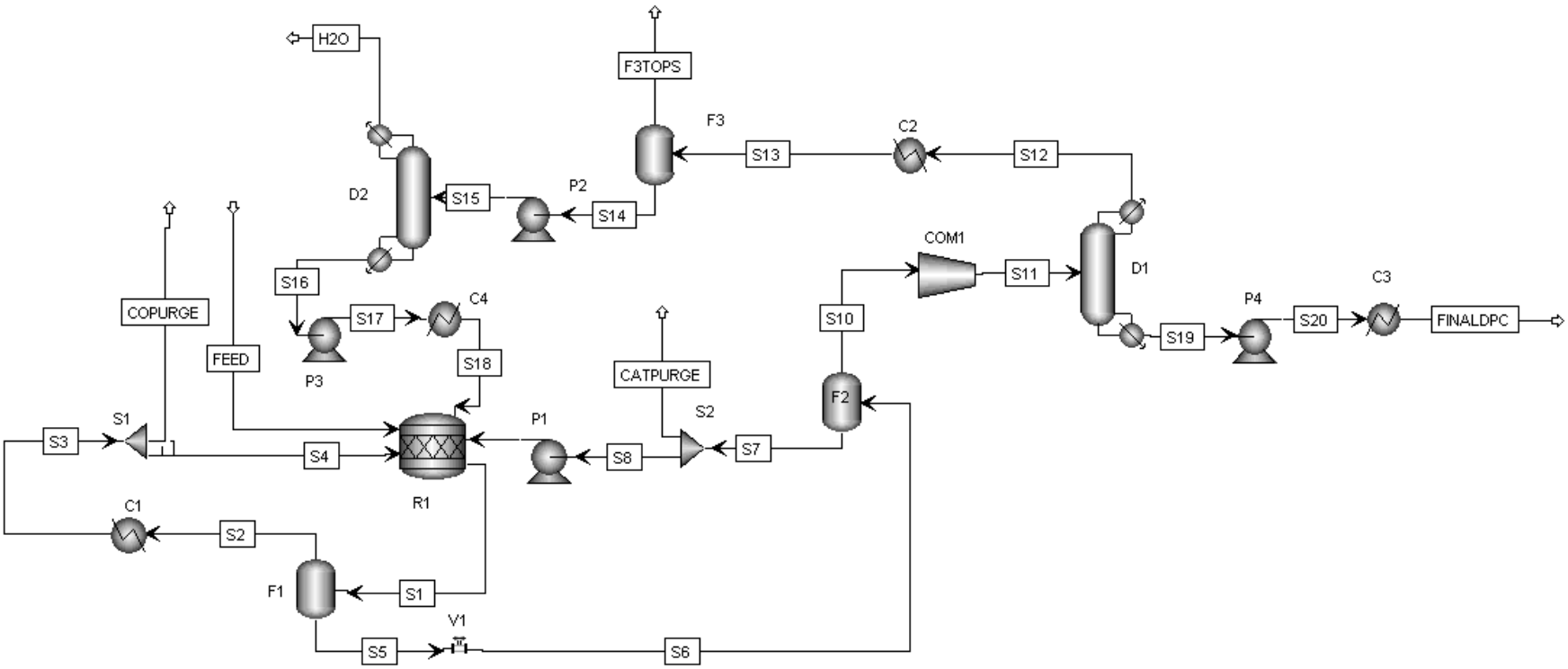


Figure 9: *Detailed ASPEN Plus flowsheet of DPC production process*

Detailed Process Description

Figure 9 shows the complete ASPEN Plus flowsheet that was used to model the DPC production process described in this report. The flowsheet represents a closed-loop recycle system that is comprised of three sections, as discussed above: the reactor section, gas and catalyst recycle loops, and a separation process to isolate DPC and recycle back as much phenol and as little water as possible. This design also incorporates pumps and heat exchangers necessary to make this flow-driven process technologically feasible.

Modeling this process in ASPEN Plus is a two-step process. The first step simulated startup conditions by disconnecting all recycle loops and requiring a "full feed" stream containing only phenol, oxygen, carbon monoxide, and the catalyst mixture, the sum of which was modeled as palladium chloride in ASPEN Plus. Once that run had completed, the recycle loops were connected, and the feed was adjusted to steady-state continuous operation conditions. The process was simulated this way so as to accurately model the recycle loops, which inevitably contain some DPC and impurities, while keeping the feed free of DPC.

Another important step in modeling this process in ASPEN Plus was inputting the thermodynamic parameters and equilibrium data for DPC, which is not included in the ASPEN Plus database. Activity coefficients for DPC were calculated according to the non-random two liquid (NRTL) model and based on the data in Hwang and Park (2011). Detailed calculations of these parameters as well as the ternary phase diagrams are provided in Appendix C.

What is omitted from Figure 9 is the control system, including the control valve at the end of the product stream (FINALDPC), and the storage tanks for the reactants and product. While storage tanks will be addressed later in this report, the control system needed to maintain this process at the required temperatures, pressures, and flowrates is a future consideration should this design be seriously

considered. The vacuum system that depressurizes the second flash vessel and the first distillation tower does not appear in the diagram but will be addressed later in this report.

Reactor Block

The single reactor used in this system is a continuously stirred tank reactor (CSTR) that operates at 80°C (176°F) and 10 bar (145 psi). Under continuous operation, the feed to this reactor, which enters at 80°C (176°F) and 10 bar (145 psi), is mixed with the CO, catalyst, and phenol recycle streams. These reaction conditions, as well as the reactant proportions in the startup feed stream to the reactor, were taken from US Patent 8,212,066, on which this process is based. Oxygen and carbon monoxide initially entered at a 5/95 volumetric ratio, and oxygen was modeled as the limiting reactant. Phenol had a single-block conversion of 10%.

In the example given in this patent, the conversion of phenol was 10.3% and the selectivity for diphenyl carbonate was 99.1% when the ligand was 3,6-dibromocarbazole 60 minutes after the reaction was initiated. Using a stainless steel high pressure reactor with stirrer, the authors of the patent obtained best results at 80°C and 10 bar. It was noted that when the temperature rose above 80°C, the conversion of phenol decreased significantly. This is due to the exothermicity of the reaction. The equilibrium favors the production of diphenyl carbonate at low temperatures, but at low temperatures, the rate of the reaction would be too small to be practical. It was noted that when the pressure of the reactor fell below 10 bar, the conversion of phenol also decreased significantly. This is because the solubility of carbon monoxide and oxygen increases with increasing pressure. Taking into account these considerations, a pressurized continuous stirred tank reactor (CSTR) with an on-line heat exchanger for external cooling was envisioned as the first step in this design of the DPC production process.

Because the reactants are a mixture of gases and liquids, the carbon monoxide and oxygen are dispersed through the liquid reactants with a strong agitator driven by a motor. Since the reactor

encloses an exothermic reaction, coils remove excess heat from the vessel by acting as large scale cooling fins as per the recommendation of industrial consultants. This maintains the ideal temperature for the reaction of 80°C.

An additional repercussion of the exothermic reaction is the resultant product streams leaving at an elevated temperature. As shown in the Utilities section later in this report, the energy in the phenol recycle stream is used to heat a different part of the process so that the phenol reenters the reactor at a lower temperature and prevents a larger heat rise. It is important that the temperature and pressure conditions remain steady so that the catalysts remain in a homogeneous phase, the DPC does not decompose, and the reaction conversion remains at 10%.

Gas and Catalyst Recycle Loops

The reactor effluent passes through the first flash vessel, F1, which operates at 145 psi and 80°F to separate the gases from the liquids in the product stream. Although this block is modeled as a separate vessel in ASPEN and in these analyses, it would sit directly at the base of the reactor in a built plant. The vapor stream is condensed slightly to 77°F, and 5% of the stream is purged to remove some phenol and water from returning to the reactor while recycling as much unused CO as possible. This recycle loop was developed to recycle CO without recycling water, a byproduct of the reaction. The CO recycle stream has a total flowrate of 14,753.97, 99% of which is CO with a 1% phenol impurity.

The bottoms from F1 pass through valve V1, which reduces the pressure to 0.15 psi. This partial vacuum is maintained until after the first distillation tower, D1, so as to keep the temperature of the process low enough for DPC to remain stable. The second flash vessel, F2, isolates the catalysts from the product stream for recycle back to the reactor. The catalyst recycle stream contains 99% of the catalysts in the system, along with small amounts of phenol and DPC. To minimize the amount of DPC

recycled back into the reactor while avoiding impurity buildup in the system, the catalyst purge stream is 1% of stream S7.

Separation Train

Two distillation towers in series are used to isolate the DPC and recycle as much phenol as possible back into the reactor. The first tower, D1, operates under a partial vacuum of 0.15 psi. It is important to note that the normal boiling point of DPC is 583^{o}F, making a partial vacuum necessary for practical purposes by reducing the amount of coking and decomposition inside the distillation column. The bottom product of D1, stream S19, contains 12749.56 lb/hr of DPC and 250.19 lb/hr of phenol and is 98% pure DPC, sufficient for the consumer. Stream S19, which is at 1.01 psi and 400^{o}F, is then pumped and condensed to 14.5 psi and 212^{o}F before entering storage tanks.

The tops product of D1, stream S12, is mostly phenol with some water and carbon monoxide and exits the tower at 0.48 psi and 191^{o}F. It passes through C2, which cools it to 77^{o}F, before passing through F3, which removes over 99% of the CO in F3TOPS. Stream S14, which contains about 99% phenol but whose flowrate is 111,630.25 lb/hr, passes through tower D2. 99.7% of the water that enters D2 is removed in the top stream H2O, and the phenol and remaining water is returned to 145 psi before reentering R1.

Although not shown in the process flow diagram, two storage tank vessels are required for proper operation of this plant. The first storage vessel, ST1, holds the phenol that is fed into the reactor at a constant temperature of 113^{o}F. This vessel is designed to contain seven days' worth of phenol to insure that the plant would still be able to operate in the event of missed deliveries from suppliers. The vessel also ensures continuous input into the reactor and would be equipped with a control valve to avoid fluctuations in phenol concentration. The second storage vessel, ST2, stores seven days' worth of

DPC product at 212^{o}F. This would insure that customers would still be able to obtain their purchased DPC in the event of a plant shutdown.

As mentioned above, the vacuum system that maintains F1 and D1 at a partial vacuum is also not shown in Figure 9. However, the economic analysis of including such an important component in this process is discussed in a later section in this report.

Energy Balance and Utility Requirements

Energy Balance

One of the major concerns in this process is the amount of heating and cooling needed, primarily in the use of flash vessels and distillation columns. Distillation is both energy intensive and thermodynamically inefficient, but it was deemed the best separation method to isolate nearly pure DPC while using the least amount of material and energy.

One way to reduce the energy requirement is to exchange heat from hot process streams that need to be cooled to cold process streams that need to be heated. This process, however, runs under relatively low temperatures, and a careful design of the heat exchanger network was necessary to best utilize the heat already in the process. Figure 10, presented on the next page, shows the process flow diagram for the heat exchanger network as modeled in ASPEN Plus.

Hot Utilities

Table VI lists all of the process units that require heating. It can be seen that a considerable amount of heating is required for the flash vessel F2, because most of the process stream entering F2 must be vaporized and separated from the homogeneous catalyst, which remains in solution and is recycled back to the reactor.

Table VI: *Process units that require heating*

Block	Stream in	Stream out	Temp in (°C)	Temp out (°C)	Heat duty (MMBtu/hr)
F2	FLASHED	CAT, F2TOPS	57	120	33.367
D1 (reboiler)	-	DPC	-	205.222	10.947
D2 (reboiler)	-	PHOH	-	193.142	19.355

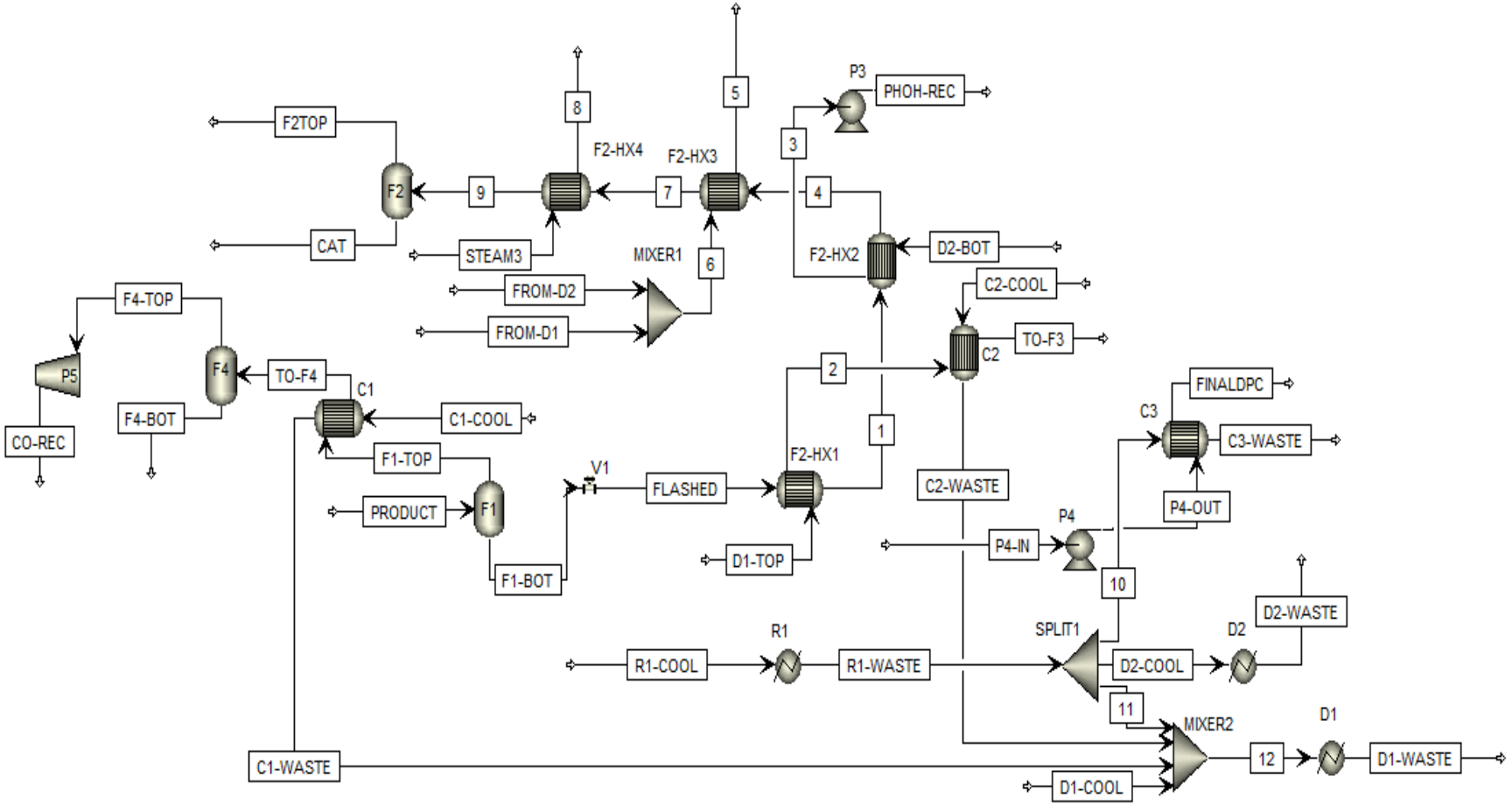


Figure 10: *Heat exchanger network for DPC production process*

***Table VII**: Material flow in the heat exchanger network*

	1	2	3	4	5	6	7	8	9	10	11	12
Temperature C	73.1	83.1	90.4	80.4	122.7	214.1	112.7	130	120	70	70	47.6
Pressure bar	0.01	0.03	1.37	0.01	20.64	20.64	0.01	3.44	0.01	3.45	3.45	3.45
Vapor Frac	0.703	0.314	0	0.813	0	0	0.983	0	0.999	0	0	0
Mole Flow kmol/hr	588.866	563.273	117.872	588.866	930.875	930.875	588.866	29.975	588.866	205.89	1644.528	10600.52
Mass Flow kg/hr	56154.72	50266.4	11087.12	56154.72	16769.97	16769.97	56154.72	540	56154.72	3709.171	29626.64	190971.3
Mole Flow kmol/hr												
PHENOL	526.822	525.779	117.791	526.822	0	0	526.822	0	526.822	0	0	0
WATER	26.549	26.664	0.081	26.549	930.875	930.875	26.549	29.975	26.549	205.89	1644.528	10600.52
DPC	27.265	0	0	27.265	0	0	27.265	0	27.265	0	0	0
CO	8.065	10.83	0	8.065	0	0	8.065	0	8.065	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0.165	0	0	0.165	0	0	0.165	0	0.165	0	0	0
Mole Frac												
PHENOL	0.895	0.933	0.999	0.895	0	0	0.895	0	0.895	0	0	0
WATER	0.045	0.047	0.001	0.045	1	1	0.045	1	0.045	1	1	1
DPC	0.046	0	0	0.046	0	0	0.046	0	0.046	0	0	0
CO	0.014	0.019	0	0.014	0	0	0.014	0	0.014	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0	0	0	0	0	0	0	0	0	0	0	0

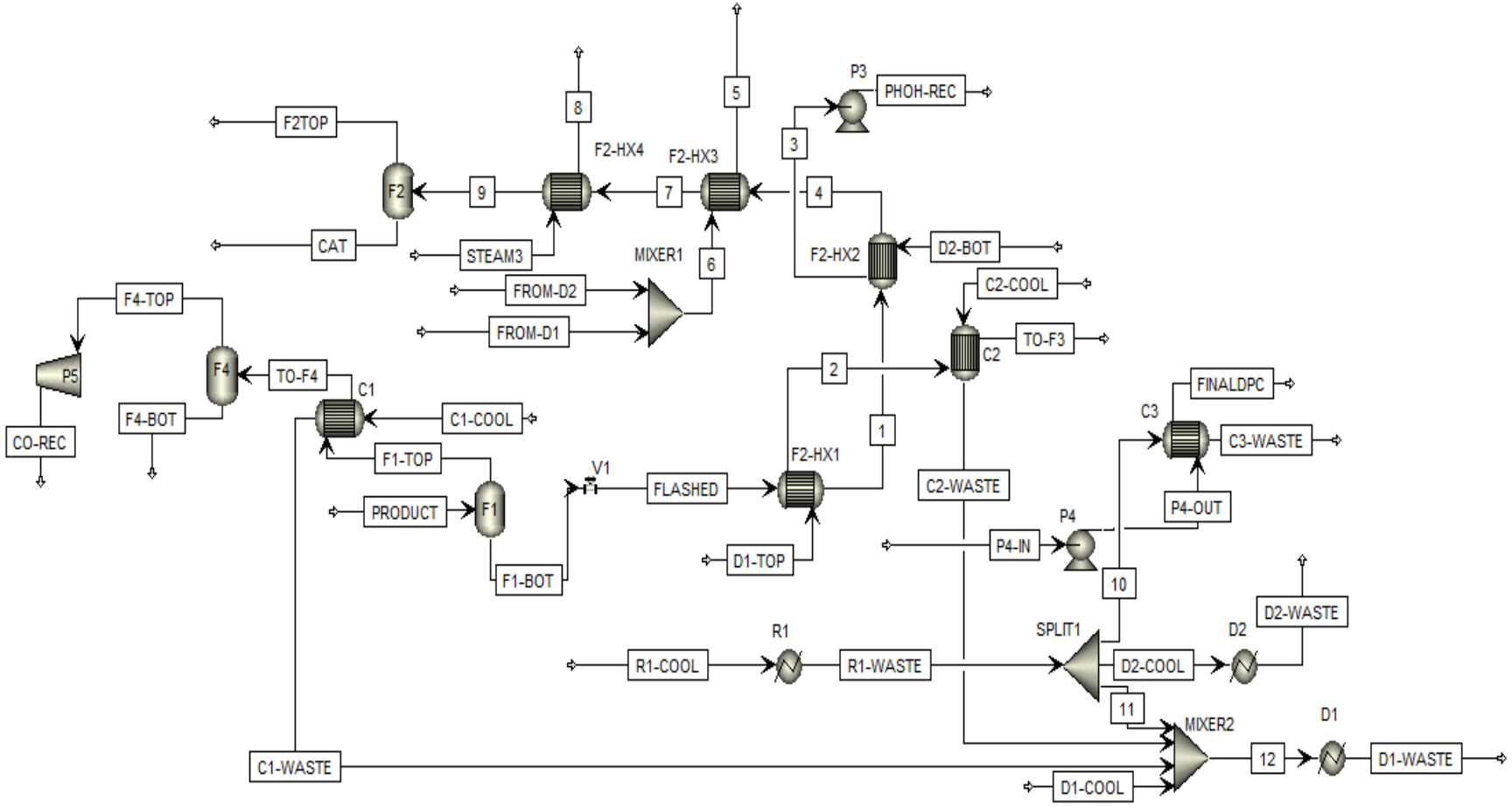


Figure 10: *Heat exchanger network for DPC production process*

***Table VII (continued)**: Material flow in the heat exchanger network*

	C1-COOL	C1-WASTE	C2-COOL	C2-WASTE	C3-WASTE	CAT	CO-REC	D1-COOL	D1-TOP	D1-WASTE	D2-BOT	D2-COOL
Temperature C	20	60	20	65	138.1	120	29.2	20	88.2	75	193.2	70
Pressure bar	3.45	3.45	3.45	3.45	3.45	0.01	10	3.45	0.03	3.45	1.37	3.45
Vapor Frac	0	0	0	0	0	0	1	0	1	0	0.28	0
Mole Flow kmol/hr	129.37	129.37	4429.957	4429.957	205.89	0.633	204.52	4396.66	563.273	10600.52	117.872	972.363
Mass Flow kg/hr	2330.636	2330.636	79806.91	79806.91	3709.171	106.893	5724.116	79207.06	50266.4	190971.3	11087.12	17517.38
Mole Flow kmol/hr												
PHENOL	0	0	0	0	0	0.189	0.006	0	525.779	0	117.791	0
WATER	129.37	129.37	4429.957	4429.957	205.89	0	0.5	4396.66	26.664	10600.52	0.081	972.363
DPC	0	0	0	0	0	0.279	0	0	0	0	0	0
CO	0	0	0	0	0	0	204.014	0	10.83	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0	0	0	0	0	0.165	0	0	0	0	0	0
Mole Frac												
PHENOL	0	0	0	0	0	0.298	0	0	0.933	0	0.999	0
WATER	1	1	1	1	1	0	0.002	1	0.047	1	0.001	1
DPC	0	0	0	0	0	0.441	0	0	0	0	0	0
CO	0	0	0	0	0	0	0.998	0	0.019	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0	0	0	0	0	0.261	0	0	0	0	0	0

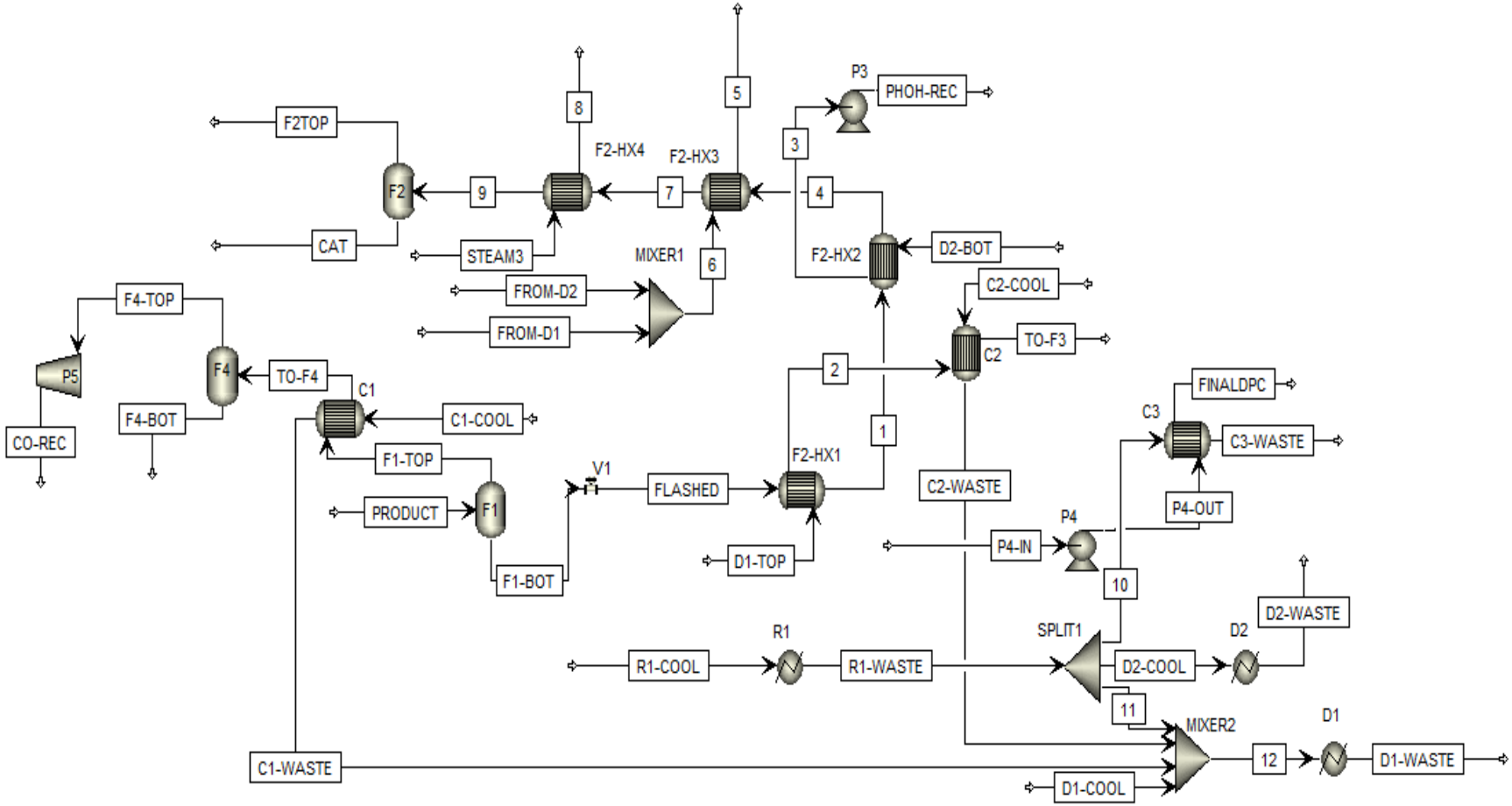


Figure 10: *Heat exchanger network for DPC production process*

Table VII (continued): *Material flow in the heat exchanger network*

	D2-WASTE	F1-BOT	F1-TOP	F2TOP	F4-BOT	F4-TOP	FINALDPC	FLASHED	FROM-D1	FROM-D2	P4-IN	P4-OUT
Temperature C	85	80	80	120	25	25	100	57.1	214.1	214.1	205.6	205.7
Pressure bar	3.45	10	10	0.01	9.66	9.66	1.01	0.01	20.64	20.64	0.07	1.01
Vapor Frac	0	0	1	1	0	1	0	0.096	0	0	0	0
Mole Flow kmol/hr	972.363	588.866	205.245	588.233	0.724	204.52	27.883	588.866	337.681	593.194	27.883	27.883
Mass Flow kg/hr	17517.38	56154.72	5764.34	56047.83	40.224	5724.116	5865.696	56154.72	6083.418	10686.55	5865.696	5865.696
Mole Flow kmol/hr												
PHENOL	0	526.822	0.361	526.633	0.355	0.006	0.892	526.822	0	0	0.892	0.892
WATER	972.363	26.549	0.851	26.549	0.352	0.5	0	26.549	337.681	593.194	0	0
DPC	0	27.265	0	26.986	0	0	26.991	27.265	0	0	26.991	26.991
CO	0	8.065	204.033	8.065	0.018	204.014	0	8.065	0	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0	0.165	0	0	0	0	0	0.165	0	0	0	0
Mole Frac												
PHENOL	0	0.895	0.002	0.895	0.49	0	0.032	0.895	0	0	0.032	0.032
WATER	1	0.045	0.004	0.045	0.485	0.002	0	0.045	1	1	0	0
DPC	0	0.046	0	0.046	0	0	0.968	0.046	0	0	0.968	0.968
CO	0	0.014	0.994	0.014	0.025	0.998	0	0.014	0	0	0	0
O2	0	0	0	0	0	0	0	0	0	0	0	0
PALLA-01	0	0	0	0	0	0	0	0	0	0	0	0

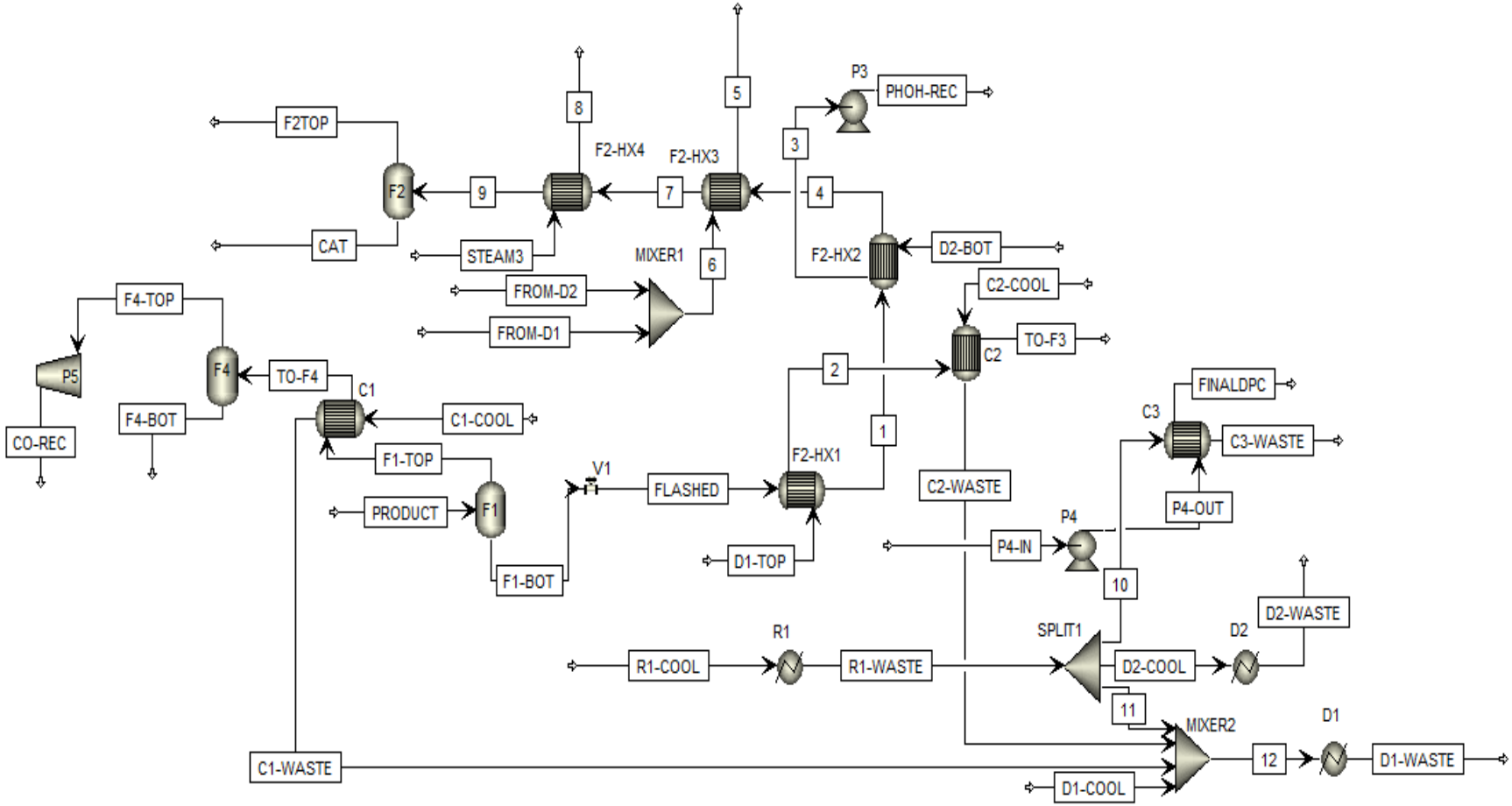


Figure 10: *Heat exchanger network for DPC production process*

Table VII (continued): *Material flow in the heat exchanger network*

	PHOH-REC	PRODUCT	R1-COOL	R1-WASTE	STEAM3	TO-F3	TO-F4
Temperature C	91.4	80	20	70	138.3	25	25
Pressure bar	10	10	3.45	3.45	3.44	0.03	9.66
Vapor Frac	0	0.258	0	0	1	0.021	0.996
Mole Flow kmol/hr	117.872	794.111	2822.781	2822.781	29.975	563.273	205.245
Mass Flow kg/hr	11087.12	61919.06	50853.2	50853.2	540	50266.4	5764.34
Mole Flow kmol/hr							
PHENOL	117.791	527.183	0	0	0	525.779	0.361
WATER	0.081	27.4	2822.781	2822.781	29.975	26.664	0.851
DPC	0	27.265	0	0	0	0	0
CO	0	212.098	0	0	0	10.83	204.033
O2	0	0	0	0	0	0	0
PALLA-01	0	0.165	0	0	0	0	0
Mole Frac							
PHENOL	0.999	0.664	0	0	0	0.933	0.002
WATER	0.001	0.035	1	1	1	0.047	0.004
DPC	0	0.034	0	0	0	0	0
CO	0	0.267	0	0	0	0.019	0.994
O2	0	0	0	0	0	0	0
PALLA-01	0	0	0	0	0	0	0

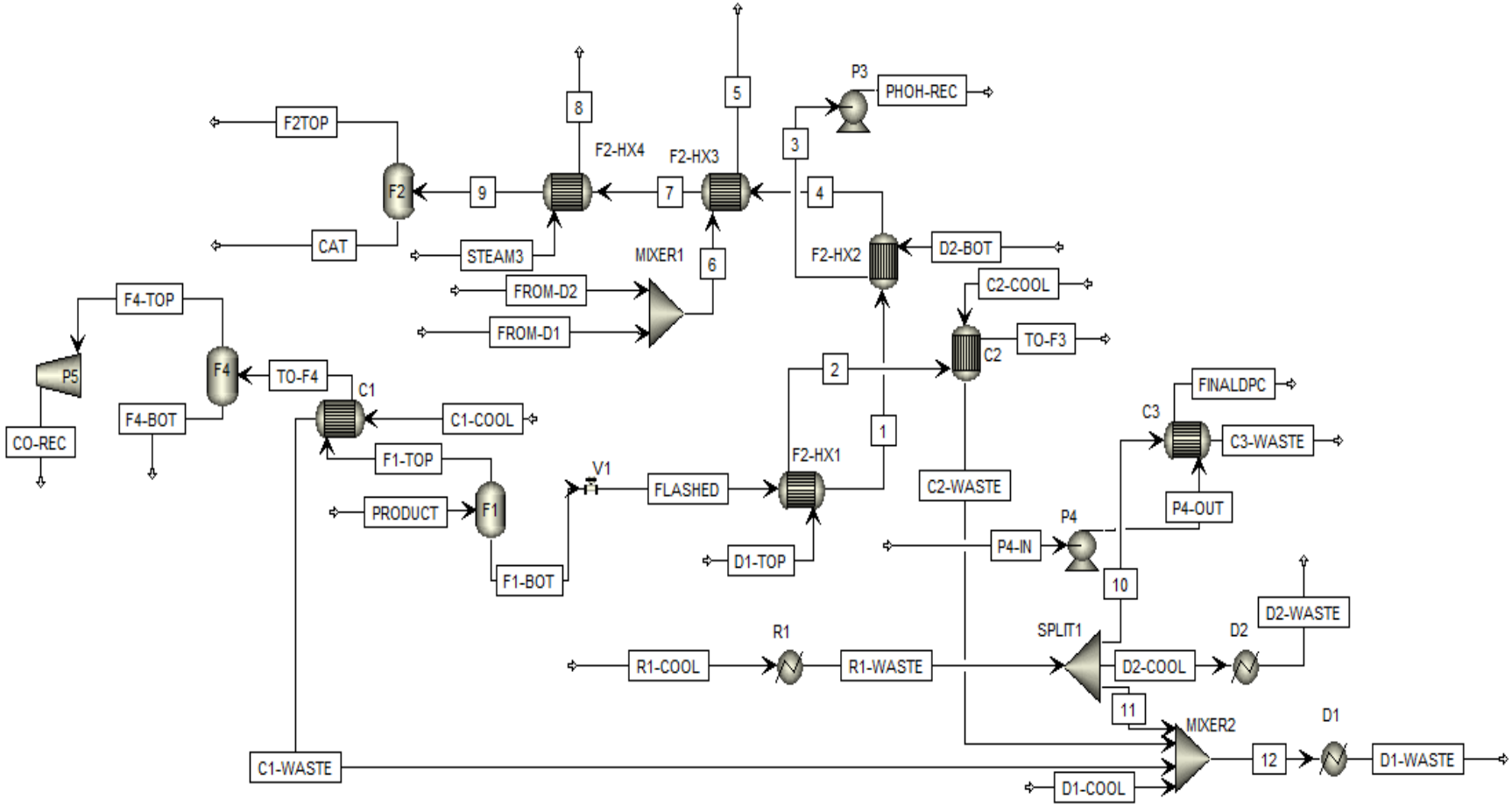


Figure 10: *Heat exchanger network for DPC production process*

Table VIII: *Heat duties and specifications for all heat exchangers in the network*

Name	C1	C2	C3	F2-HX1	F2-HX2	F2-HX3	F2-HX4	D1 condernser	D2 condenser	R1 condenser
Inlet hot stream temperature [C]	80	83.0962	205.734	88.2	193.2	214.079	138.32	-	-	80
Inlet hot stream pressure [bar]	10	0.03	1.01325	0.03	1.37	20.6421	3.43918	-	-	10
Inlet hot stream vapor fraction	1	0.314372	0	1	0.28024	3.57E-06	1	1	1	-
Outlet hot stream temperature [C]	25	25	100	83.0962	90.4211	122.682	130.022	88.3	99.7	-
Outlet hot stream pressure [bar]	9.65526	0.03	1.01325	0.03	1.37	20.6421	3.43918	0.03	1	10
Outlet hot stream vapor fraction	0.99647	0.021224	0	0.314372	0	0	0	-	-	-
Inlet cold stream temperature [C]	20	20	70	57.0503	73.0988	80.4183	112.682	-	-	20
Inlet cold stream pressure [bar]	3.44738	3.44738	3.44738	0.01	0.01	0.01	0.01	3.45	3.45	3.45
Inlet cold stream vapor fraction	0	0	0	0.096427	0.703475	0.813131	0.982708	0	0	0
Outlet cold stream temperature [C]	59.9969	64.9959	138.122	73.0988	80.4183	112.682	120.022	75	85	70
Outlet cold stream pressure [bar]	3.44738	3.44738	3.44738	0.01	0.01	0.01	0.01	3.45	3.45	3.45
Outlet cold stream vapor fraction	0	0	0	0.703475	0.813131	0.982708	0.998928	0	0	0
Heat duty [Gcal/hr]	0.087717	3.39615	0.273986	5.04074	0.980567	1.99021	0.283541	5.14461	0.267063	2.41706
Required exchanger area [sqm]	11.0928	456.325	8.09905	366.206	26.3309	40.2986	17.8627	-	-	-

As seen in Table VI, both of the distillation towers also require a considerable amount of heating. However, D1 requires less heat because it is operated under a partial vacuum. In order to supply the appropriate amount of heating for both of the distillation column reboilers, saturated steam at 300 psi was used. Thermodynamic data for saturated steam at 300 psi is shown in Table IX below. A saturated steam temperature of 214.08°C allows an ample minimum approach temperature of 13°C for D1 and 21°C for D2.

Table IX: *Properties of saturated steam at 300psi*

Property		**Metric**		**Standard**	
State		Saturated Steam			
		Use the general steam table for non-saturated steam			
Temperature (*T*)		214.08	C	417.35	F
Pressure (*P*)		20.68	bar	300	psi
Density	Saturated Liquid	847.68	kg/m^3	52.919	lb/ft^3
	Saturated Vapor	10.38		0.65	
Specific Volume	Saturated Liquid	0.00118	m^3/kg	0.0189	ft^3/lb
	Saturated Vapor	0.0964		1.54	
Enthalpy	Saturated Liquid	916.32	kJ/kg	393.95	Btu/lb
	Evaporated	1882.6		809.4	
	Saturated Vapor	2798.9		1203.3	
Entropy	Saturated Liquid	2.46	kJ/kg-K	0.59	Btu/lb-R
	Evaporated	3.86	(mayer)	0.92	
	Saturated Vapor	6.33		1.51	

Taking into account the enthalpy of condensation of saturated steam at 300psi, calculations were made in order to supply the right amount of heating for D1 and D2, and the results are shown in Table X.

Table X: *Amount of saturated steam required for D1 and D2*

	D1 (reboiler)	D2 (reboiler)
Net duty [Gcal/hr]	2.76	4.88
Net duty [kJ/hr]	11547324.6	20415904.64
Steam [kg/hr]	6133.71	10844.53
Total [kg/hr]	16978.24	

A total of approximately 17 metric tons of saturated steam per hour supplied at 300psi is needed to supply the required amount of energy for the distillation reboilers. In total, approximately 17 metric tons of saturated liquid per hour at 214.08^{o}C is available as a source of heat for the flash vessel F2.

Due to the high heat duty of the flash vessel F2, the waste heat from both distillation columns together would not be enough to supply the appropriate amount of heat needed by F2. However, two alternative sources of heat recovery were identified: (1) the vapor distillate from the distillation column D1 that needs to be cooled and condensed so that it can be pumped to column D2; and (2) the bottoms product from column D2 that needs to be cooled in order to reduce the heat duty of the reactor R1. In order to supply the remaining amount of heat for the flash vessel F2, saturated steam at 50 psi was used. Thermodynamic data for saturated steam at 50 psi is shown in Table XI below. A steam temperature of 138.32^{o}C allows an ample minimum approach temperature of 18^{o}C.

Table XI: *Thermodynamic data for saturated steam at 50 psi*

Property		Metric		Standard	
State		Saturated Steam			
		Use the general steam table for non-saturated steam			
Temperature (T)		138.32	C	280.98	F
Pressure (P)		3.45	bar	50	psi
Density	Saturated Liquid	927.62	kg/m^3	57.91	lb/ft^3
	Saturated Vapor	1.88		0.12	
Specific Volume	Saturated Liquid	0.0011	m^3/kg	0.017	ft^3/lb
	Saturated Vapor	0.532		8.52	
Enthalpy	Saturated Liquid	581.98	kJ/kg	250.21	Btu/lb
	Evaporated	2149.3		924	
	Saturated Vapor	2731.3		1174.2	
Entropy	Saturated Liquid	1.7219	kJ/kg-K	0.41	Btu/lb-R
	Evaporated	5.22	(mayer)	1.25	
	Saturated Vapor	6.95		1.66	

The effort to reduce the heat duty of F2 was successful, reducing the amount of saturated steam required by about 96%, as shown in Table XII:

Table XII: *Amount of steam required for F2 with and without heat recovery*

	Without heat recovery	**With heat recovery**
Net duty [Gcal/hr]	8.40839	0.283541
Net duty [kJ/hr]	35195838.86	1186845.918
Steam [kg/hr]	16375.48916	552.20114

Referring to Figure 10, the bottoms product from the disengagement vessel F1 is subject to a pressure reduction by passing through a relief valve V1. The stream FLASHED then enters the first heat exchanger, F2-HX1, where heat is provided by the partial latent heat of condensation of the distillate

from the column D1. The stream then enters the second heat exchanger, F2-HX2, where heat is provided by cooling the bottoms product from the distillation column D2. Here, both the distillate from D1 and the bottoms product from D2 need to be cooled. Stream FLASHED then enters a third heat exchanger, F2-HX3, where heat is provided by cooling the saturated liquid obtained from the reboilers of columns D1 and D2. At this point, the temperature of the stream FLASHED is 112^{o}C, close to the specified temperature of 120^{o}C for flash vessel F2. A last heat exchanger, F2-HX4 supplies the remaining heat by using saturated steam at 50 psi, as explained above. All heat exchangers were designed with a minimum approach temperature of 10^{o}C to maintain practical heat exchanger sizes.

As shown by Table XII, approximately 0.55 metric tons of saturated steam at 50 psi per hour is needed to supply the right amount of heat for the vacuum flash vessel F2. This is significantly lower than the 16.4 metric tons of saturated steam at 50 psi per hour needed if no heat exchangers were used in this process.

Cold Utilities

In addition to reducing the amount of hot utilities required in this process, the amount of cold utilities required was also reduced. Table XIII shows that a significant heat duty is also required by the condenser units in this process in order to achieve the desired changes in temperature and physical phase.

Table XIII: *Process units that require cooling*

Block	Temp in (^{o}C)	Temp out (^{o}C)	Heat duty (MMBtu/hr)
R1	-	80	-9.592
C1	80	25	-0.426
C2	88.3	25	-33.966
C3	205.1	100	-1.091
D1 (condenser)	-	88.3	-20.415
D2 (condenser)	-	99.7	-1.060

However, it became apparent that the use of cooling water would require an exorbitant amount of water being pumped to the system, as illustrated in Table XIV. As the amount of cooling water increases, the energy input required in the pumps and the cost of the heat exchangers also increase. Moreover, mineral deposition from cooling water causes severe problems in the heat exchangers, requiring routine cleaning maintenance operations that result in more frequent start-up operations. Therefore, the amount of cooling water required in the system was decreased by reusing and recycling deionized water obtained from distilled water or steam. Ideally, steam obtained from a nearby power plant would be cooled using a cooling tower and brought to ambient temperature.

Table XIV: *Amount of cooling water required.* $T_{in} = 20^{o}C$, $T_{out} = 45^{o}C$

	R1	C1	C2	C3	D1	D2
Net duty [Gcal/hr]	-2.41706	-0.107387	-8.559	-0.275	-5.145	-0.267
Net duty [kJ/hr]	10117329.75	449500.50	35827183.08	1150479.69	21534308.54	1117872.305
Cooling water [kg/hr]	96786.45	4300.10	342737.26	11005.95	206005.87	10694.017
Total [kg/hr]	671529.7					

Condensers C1 and C2 require the use of fresh coolant (C1-COOL and C2-COOL, respectively), which are assumed to be at $20^{o}C$. Since a large amount of heat must be removed from the reactor, fresh coolant was also used for R1 (R1-COOL). The coolant used from these three process units are then reused in C3 and in the condensers for D1 and D2. The coolant used for the reactor could alone satisfy the cooling requirements for C3 and the condenser for D2, because these last three units operate at higher temperatures and therefore the use of room temperature water is not critical. Because the heat

duty on the condenser for D1 is significantly higher than that of either C3 or D2, fresh coolant, labeled D1-COOL in Figure 10, is needed there.

This heat exchange network design resulted finally in a 68% reduction in the amount of water required for cooling. A summary of the total amount of hot and cold utilities needed in the process is summarized in Table XV below.

Table XV: *Summary of hot and cold utilities*

	Temperature (^{o}C)	Pressure (psi)	Flowrate (kg/hr)	Total (kg/hr)
Steam 1: D1 reboiler	214.08	300	6083.41751	16770
Steam 2: D2 reboiler	214.08	300	10686.5524	
Steam 3	138.32	50	552.20114	552.20114
C1-COOL	25	50	2330.63636	212197.8
C2-COOL	25	50	79806.9113	
R1-COOL	25	50	50853.1959	
D1-COOL	25	50	79207.0632	

Storage Tanks

Both storage vessels ST1 and ST2 must be heated and heavily insulated with fiberglass in order to maintain their desired temperatures of 113^{o}F and 212^{o}F, respectively. A heat exchanger, pump, and mixer on each tank would ensure a uniform temperature throughout. With a 3-inch jacket of fiberglass on each tank and an outdoor temperature of 86^{o}F, the estimated energy requirements for the tanks are summarized in Table XVI.

Table XVI: *Estimated energy requirements needed to maintain heated storage units*

Vessel	Sustained Temperature (^{o}F)	Energy Requierment (kW)
ST1	113	7.77
ST2	212	12.02

Electricity

All pumps, motors, and compressors used in this process are powered by electricity. The work required by each pump was calculated in ASPEN Plus. The total electric utility requirement of all pumps, motors, and compressors is 1351.48 kWh, and a detailed electric utility cost calculation is found in Table XXXIV in Appendix G.

Equipment List and Unit Descriptions

Unit Descriptions

The following is a list of all units that appear in the DPC production process as well as in the heat exchanger network. Detailed sizing and costing information can be found in the Appendix and the relevant unit specification sheets in the following section.

Process Equipment

Reactor R1

Reactor R1 is a continuous stirred tank reactor (CSTR) that operates at 80°C (176°F) and 10 bar (145 psi). The reactor feed is comprised of fresh feed and recycled CO, catalysts, and phenol, as well as some water and DPC impurities in the recycle streams. The liquid feed is fed into the reactor through pipes, and the gas feed is bubbled in and incorporated with an agitator. Cooling coils are used to remove the heat associated with the agitator and motor. The reactor is made of stainless steel to avoid corrosion and reduce fouling and has an inner diameter of 26.7 ft and a length of 53.4 ft. The reactor's bare module cost is $1,942,684.69, the agitator's bare module cost is $199,950.00, the steam turbine motor's bare module cost is $122,249.38, and the cooling coils' bare module cost is $63,694.58; the total bare module cost for the entire reactor system is $2,328,578.65.

Flash Vessel F1

Flash vessel F1 separates the gases from the liquids in the reactor effluent. Although it is listed in this report as a separate piece of equipment, it would sit directly at the reactor outlet in an actual facility. Carbon monoxide, unreacted oxygen, and small amounts of water and phenol exit through the top, and phenol, DPC, water, and the catalyst mixture exit through the bottom. F1 operates at 176°F and 145 psi and is made of stainless steel to avoid corrosion and reduce fouling. F1 has an inner diameter of 5.2 ft and a height of 13.1 ft. The bare module cost of F1 is $743,308.57.

Condenser C1

Condenser C1 cools the gaseous stream leaving F1 from 176°F to 77°F before returning most of the unused carbon monoxide to the reactor. In the shell side, cooling water enters at 68°F and exits at 140°F. C1 is modeled as a countercurrent shell and tube heat exchanger with a heat transfer area of 119.37 ft^2 and an overall heat duty of 425,930 BTU/hr. The bare module cost of C1 is $124,002.54.

Splitter S1

Splitter S1 is used to split stream S3 into COPURGE, which removes some impurities from the system, and S4, which recycles most of the unused CO back into reactor R1.

Valve V1

Valve V1 is used to lower the pressure of stream S5, the bottoms of F1, from 145 psi to 0.145 psi. This partial vacuum is necessary to prevent the temperature later in the process from becoming high enough to cause DPC to decompose.

Flash Vessel F2

Flash vessel F2 separates the catalyst mixture from DPC, phenol, and water. The catalyst mixture exits through the bottom of F2, and the DPC, phenol, and water stream exits through the top. F2 operates at 248°F and 0.145 psi and is made of stainless steel to avoid corrosion and reduce fouling. F1 has an inner diameter of 1.06 ft and a height of 4.59 ft. The bare module cost of F2 is $103,889.53.

Splitter S2

Splitter S2 is used to split stream S7 into S8, which recycles 99% of the catalyst mixture back to reactor R1, and CATPURGE, which purges a small amount of catalyst and prevents the buildup of impurities in the system.

Pump P1

Pump P1 is a centrifugal pump that raises the pressure of the catalyst recycle stream from 0.145 psi to 203 psi before it reenters reactor R1. The pump efficiency is 0.296, and it consumes 123 W of electricity. The bare module cost of P1 is $11,479.12, and the bare module cost of its electric motor is $10,435.39; all together, the bare module cost of P1 is $21,914.52.

Compressor COM1

Compressor COM1 compresses the DPC, phenol, and water stream that exits F2 from 248^{o}F and 0.145 psi to 388^{o}F and 1.45 psi before it enters distillation column D1. It is made of stainless steel and operates at 72% efficiency. The bare module cost of COM1 is $4,371,110.81.

Distillation Tower D1

Distillation tower D1 is a 14-stage packed tower that separates DPC from phenol and water. The feed enters on tray 5, and the molar reflux ratio is 0.65. The column operates under a partial vacuum to prevent the DPC from decomposing; the top stage pressure is 25 mmHg, the condenser pressure drop is 25 mmHg, and each stage sustains a 7.5 mmHg pressure drop. The column diameter is 11.67 ft, and the column is made of Mellapak standard packing with a HETP of 17 inches. A detailed description of the optimization of D1 is given in Appendix E. The bare module cost of the column is $3,719,952.70, the bare module cost of the condenser is $57,400.00, the bare module cost of the reboiler is $76,300.00, the bare module cost of the reboiler pump is $87,744.73, the bare module cost of the reboiler motor is

$236,535.55, the bare module cost of the reflux accumulator is $102,100.00, and the bare module cost of the reflux pump and motor is $27,400.00; all together, the bare module cost of D1 is $4,307,432.98.

Condenser C2

Condenser C2 cools the distillate from D1 from 176^{o}F to 77^{o}F before the phenol and water mixture is separated. In the shell side, cooling water enters at 68^{o}F and exits at 149^{o}F. C2 is modeled as a countercurrent shell and tube heat exchanger with a heat transfer area of 4911.57 ft^{2} and an overall heat duty of 33,969,000 BTU/hr. The pressure drop across the condenser is 5 psi. The bare module cost of C2 is $121,571.12.

Flash Vessel F3

Flash vessel F3 removes some water and carbon monoxide from stream S13 before removing as much phenol as possible to recycle into R1. F3 operates at 77^{o}F and 0.48 psi. F3 has an inner diameter of 0.55 ft and a height of 4.02 ft. The bare module cost of F2 is $104,300.00.

Vacuum System

A vacuum system keeps blocks F2, COM1, D1, C2, and F3 under a partial vacuum so that the temperature does not reach the boiling point of DPC. Calculating the air leakage at each major unit block within the system is critical to maintaining steady operation of this vacuum, and these calculations are based on the size and volume of the vessels using a correlation table provided by Mr. Fabiano. The most efficient pump necessary for the range of flowrates and horsepower required for this system is a stainless steel, oil sealed, liquid ring pump that draws a vacuum at 22.5 Torr. This pump cools the vapor effluent stream leaving F3 after it is saturated with oil. The effluent mixer is then sent through a separation scheme that includes further cooling, flash separation, and the recirculation and recycle of oil

into the pump. A major producer of this pump type is Nash-Kinema, who offers liquid ring pumps with various numbers of stages based on horsepower requirements. The bare module cost of the vacuum pump is $47680.18, and the utility cost associated with this unit is $219,797.07.

Pump P2

Pump P2 is a centrifugal pump that raises the pressure of stream S14 from 0.48 psi to 20.3 psi at 77^{o}F before it enters distillation tower D2. The pump efficiency is 0.622, and it consumes 2.84 kW of electricity. The bare module cost of P2 is $16,189.43, and the bare module cost of its electric motor is $3,478.46; all together, the bare module cost of P2 is $19,667.89.

Distillation Tower D2

Distillation tower D2 is an 11-stage tray tower that separates water from phenol, which is recycled back to reactor R1. The feed enters on tray 8, and the molar reflux ratio is 1.02. The top stage pressure is 1 bar, the condenser pressure drop is 200 mmHg, and each stage sustains an 8.5 mmHg pressure drop. The column diameter is 6.80 ft, and the column is made of Koch Flexitray trays with a tray spacing of 2 ft. A detailed description of the optimization of D2 is given in Appendix E. The bare module cost of the column is $1,125,809.20, the bare module cost of the condenser is $43,800.00, the bare module cost of the reboiler is $59,600.00, the bare module cost of the reboiler pump is $25,871.01, the bare module cost of the reboiler motor is $23,189.76, the bare module cost of the reflux accumulator is $101,400.00, and the bare module cost of the reflux pump is $26,000.00; all together, the bare module cost of D2 is $1,405,669.97.

Pump P3

Pump P3 is a centrifugal pump that raises the pressure of stream S16 from 19.85 psi to 145 psi at 380°F before it is cooled by condenser C4 and recycled back to reactor R1. The pump efficiency is 0.639, and it consumes 20.43 kW of electricity. The bare module cost of P3 is $12,153.95, and the bare module cost of its electric motor is $1,739.23; all together, the bare module cost of P3 is $13,893.18.

Condenser C4

Condenser C4 cools stream S17 from 380°F to 194°F before recycling the unused phenol back to reactor R1. It is modeled as a heater, and its heat duty is 11,261,000 BTU/hr. The bare module cost of C4 is 91,236.

Pump P4

Pump P4 is a centrifugal pump that raises the pressure of the DPC stream from the bottom of D1 from 1.01 psi to 19.5 psi at 401°F before it is cooled by condenser C3 and sent to storage tanks. He pump efficiency is 0.326, and it consumes 20.43 kW of electricity. The bare module cost of P4 is $15,967.60, and the bare module cost of its electric motor is $2,496.22; all together, the bare module cost of P3 is $18,463.82.

Condenser C3

Condenser C3 cools the DPC product stream S20 from 401°F to 212°F before sending the product to storage tanks. C3 is modeled as a countercurrent shell and tube heat exchanger with a heat transfer area of 87.0 ft^2 and a heat duty of 11,261,000 BTU/hr. The pressure drop across the condenser is 5 psi. The bare module cost of C4 is $91,236.

Storage Tanks ST1 and ST2

Storage tank ST1 stores one week's supply of phenol at 113°F before it enters reactor R1, and storage tank S2 stores one week's production of DPC at 212°F to be delivered to the customer. Both tanks are made of Incoloy-825 and have a wall thickness of 0.625 inches.. To maintain the tanks at their uniform desired temperatures, each tank is fitted with a heat exchanger, pump, and mixer and is insulated by three inches of fiberglass to maintain a constant temperature. ST1 holds a capacity of 288,272 gallons and has an inner diameter of 25.4 ft, and ST2 holds a capacity of 54,974 gallons and has an inner diameter of 14.61 ft; a more detailed explanation of tank sizing and costing can be found in the Appendix. The bare module cost for ST1 is $3,753,232.61, and the bare module cost for ST2 is $1,601,920.65.

Heat Exchanger Network Equipment

Heat Exchanger F2-HX1

Heat exchanger F2-HX1 heats the liquid bottoms product from F1 with the latent heat in the distillate stream from D1. The minimum approach temperature difference in designing this heat exchanger was 18°F. F2-HX1 is modeled as a countercurrent shell and tube heat exchange with a heat transfer area of 3941.85 ft^2 and a heat duty of 5.04 Gcal/hr. The bare module cost of F2-HX1 is $194,700.25.

Heat Exchanger F2-HX2

Heat exchanger F2-HX2 further heats the liquid bottoms product from F1 with the latent heat in the bottoms stream from D2. The minimum approach temperature difference in designing this heat exchanger was 18°F. F2-HX2 is modeled as a countercurrent shell and tube heat exchange with a heat transfer area of 283.4 ft^2 and a heat duty of 0.98 Gcal/hr. The bare module cost of F2-HX2 is $71,008.06.

Heat Exchanger F2-HX3

Heat exchanger F2-HX3 further heats the liquid bottoms product from F1 with the heat from cooling the saturated liquid from the reboilers of both columns D1 and D2. The minimum approach temperature difference in designing this heat exchanger was 18^{o}F. F2-HX3 is modeled as a countercurrent shell and tube heat exchange with a heat transfer area of 433.77 ft^2 and a heat duty of 1.99 Gcal/hr. The bare module cost of F2-HX3 is $76,806.16.

Heat Exchanger F2-HX4

Heat exchanger F2-HX4 further heats the liquid bottoms product from F1 with 50 psi steam. The minimum approach temperature difference in designing this heat exchanger was 18^{o}F. F2-HX4 is modeled as a countercurrent shell and tube heat exchange with a heat transfer area of 192.27 ft^2 and a heat duty of 0.284 Gcal/hr. The bare module cost of F2-HX4 is $68,010.05.

Flash Vessel F4

Flash vessel F4 separates CO from water and phenol to be recycled back to reactor R1. The bare module cost of F4 is $47,995.78.

Unit Specification Sheets

Reactor: R1

R1					
Block Type:	Reactor				
Function:	Produces DPC				
Materials:	In (1)	In (2)	In (3)	In (4)	Out
Stream	FEED	S4	S9	S18	S1
Mass Flow (lb/Hr)	15400	8232.23	889310	2136.02	913050
Volumetric Flow (ft3/Hr)	6433.04	13857	12287	31.69	25812
Breakdown(lb/Hr):					
Phenol	11502	0.235	23382	629.92	24260
Water	0	37.243	16.807	30.4	1159
DPC	0	0.7	865860	1475.69	878420
CO	2944.67	8194	0.2056	0	9163.7
O_2	952.4	0	0	0	0
Catalyst Mix	0.646	0	52.78	0	53.32
Operating Conditions:					
Operating Pressure (psia)	145.04				
Operating Temperature (^oC)	80				
Design Data:					
Construction Material	Stainless Steel 316				
Weight (lb)	256,643				
Volume (ft^3)	29951				
Diameter (ft)	26.72				
Length (ft)	53.43				
Wall Thickness (in)	0.5				
Purchase Cost:	$873,645.46				
Bare Module Cost:	$2,664,618.64				

Pump: P1		
Block Type:	Centrifugal Pump	
Function:	Pumps catalyst recycle stream	
Materials:	Inlet	Outlet
Stream	S8	S9
Operating Conditions:		
Presssure Increase (psi)	202.9	
Pressure Head (ft-lbf/Lb)	423.29	
Flow Rate (ft^3/Hr)	3.3	
Design Data:		
Construction Material	Chloride resitant	
Number of Stages	1	
Pump Efficiency	0.296	
Consumed Power (kW)	0.123	
Power Source	Electricity	
Purchase Cost:	$3,478	
Bare Module Cost:	$11,479	

Pump: P2		
Block Type:	Centrifugal Pump	
Function:	Pumps F3 distillate	
Materials:	Inlet	Outlet
Stream	S14	S15
Operating Conditions:		
Presssure Increase (psi)	19.82	
Pressure Head (ft-lbf/Lb)	42.06	
Flow Rate (ft^3/Hr)	1,645	
Design Data:		
Construction Material	Stainless steel	
Number of Stages	1	
Pump Efficiency	0.622	
Consumed Power (kW)	2.841	
Power Source	Electricity	
Purchase Cost:	$4,905.90	
Bare Module Cost:	$16,189	

Pump: P3		
Block Type:	Centrifugal Pump	
Function:	Pumps Phenol recycle stream	
Materials:	Inlet	Outlet
Stream	S16	S17
Operating Conditions:		
Presssure Increase (psi)	125.18	
Pressure Head (ft-lbf/Lb)	313.8	
Flow Rate (ft^3/Hr)	1,925	
Design Data:		
Construction Material	Stainless steel	
Number of Stages	1	
Pump Efficiency	0.639	
Consumed Power (kW)	20.43	
Power Source	Electricity	
Purchase Cost:	$3,683	
Bare Module Cost:	$12,153	

Pump: P4		
Block Type:	Centrifugal Pump	
Function:	Pressurizes product stream	
Materials:	Inlet	Outlet
Stream	S19	S20
Operating Conditions:		
Presssure Increase (psi)	18.487	
Pressure Head (ft-lbf/Lb)	39.541	
Flow Rate (ft^3/Hr)	193.1	
Design Data:		
Construction Material	Stainless steel	
Pump Efficiency	0.326	
Consumed Power (kW)	20.43	
Power Source	Electricity	
Purchase Cost:	$3,165.70	
Bare Module Cost:	$15,967.60	

Condenser: C1		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Condenses gas recycle stream	
Tube:	Inlet	Outlet
Stream	S2	S3
Temperature (^oC)	80	25
Pressure (bar)	10	10
Shell:	Inlet	Outlet
Stream	C1-COOL	C1-WASTE
Temperature (^oC)	20	60
Pressure (bar)	3.45	3.45
Operating Conditions:		
Tube Flow Rate (lb/h)	8232.23	
Shell Flow Rate (lb/h)	2330.63	
Design Data:		
Construction Material	Carbon Steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	119.372	
Heat Duty (BTU/Hr)	425,930	
Purchase Cost:	$38,350.51	
Bare Module Cost:	$124,002.54	

Condenser: C2		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Condenses distillate from D1	
Tube:	Inlet	Outlet
Stream	S12/2	S13/TO-F3
Temperature (^oC)	128.155	25
Pressure (bar)	0.033	0.033
Shell:	Inlet	Outlet
Stream	C2-COOL	C2-WASTE
Temperature (^oC)	20	65
Pressure (bar)	3.45	3.45
Operating Conditions:		
Tube Flow Rate (lb/h)	4,191.57	
Shell Flow Rate (lb/h)	175,944	
Design Data:		
Construction Material	Carbon Steel	
Flow Direction	Countercurrent	
Transfer Area(f^2)	4911.57	
Heat Duty (BTU/Hr)	33,969,000	
Purchase Cost:	$38,350.51	
Bare Module Cost:	$121,571.12	

Condenser: C3		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Cools down product stream	
Tube:	Inlet	Outlet
Stream	S20	FINALDPC
Temperature (^oC)	120	100
Pressure (bar)	0.01	1
Shell:	Inlet	Outlet
Stream	10	C3-WASTE
Temperature (^oC)	70	138.1
Pressure (bar)	3.45	3.45
Operating Conditions:		
Tube Flow Rate (lb/h)	8177.3	
Shell Flow Rate (lb/h)	2339.64	
Design Data:		
Construction Material	Carbon Steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	87.0	
Heat Duty (BTU/Hr)	1,090,700	
Purchase Cost:	$18,245.85	
Bare Module Cost:	$70,305.77	

Condenser: C4		
Block Type:	Heater	
Function:	Heats phenol recycle stream	
Materials:	Inlet	Outlet
Stream	S17	S18
Breakdown(lb/Hr):		
Phenol	110,580	
Water	3.0372	
DPC	0	
CO	9.02E-10	
O_2	0	
Catalyst Mix	0	
Design Data:		
Pressure (psia)	145	
Temperature (°F)	381	
Heat Duty (BTU/Hr)	11,261,000	
Purchase Cost:	$24,523	
Bare Module Cost:	$91,236	

Heat Exchanger: F2-HX1		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Heat Integration	
Tube:	Inlet	Outlet
Stream	D1-TOP	2
Temperature(Celcius)	88.2	83.1
Pressure(bar)	0.03	0.03
Shell:	Inlet	Outlet
Stream	FLASHED	1
Temperature(Celcius)	57.0503	73.0988
Pressure(bar)	0.01	0.01
Operating Conditions:		
Tube Flow Rate (kg/hr)	50266.396	
Shell Flow Rate (kg/hr)	56154.718	
Design Data:		
Construction Material	Stainless steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	3941.85	
Heat Duty(Gcal/hr)	5.04	
Purchase Cost:	$61,419.64	
Bare Module Cost:	$194,700.25	

Heat Exchanger: F2-HX2		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Heat Integration	
Tube:	Inlet	Outlet
Stream	D1-BOT	3
Temperature(Celcius)	193.2	90.4211
Pressure(bar)	1.37	1.37
Shell:	Inlet	Outlet
Stream	1	4
Temperature(Celcius)	73.0988	80.4183
Pressure(bar)	0.01	0.01
Operating Conditions:		
Tube Flow Rate (kg/hr)	11087.116	
Shell Flow Rate (kg/hr)	56154.718	
Design Data:		
Construction Material	Stainless steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	283.4	
Heat Duty(Gcal/hr)	0.98	
Purchase Cost:	$22,400.02	
Bare Module Cost:	$71,008.06	

Heat Exchanger: F2-HX3		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Heat Integration	
Tube:	Inlet	Outlet
Stream	6	5
Temperature(Celcius)	214.079	122.682
Pressure(bar)	20.6421	20.6421
Shell:	Inlet	Outlet
Stream	4	7
Temperature(Celcius)	80.4183	112.682
Pressure(bar)	0.01	0.01
Operating Conditions:		
Tube Flow Rate (kg/hr)	16769.97	
Shell Flow Rate (kg/hr)	56154.718	
Design Data:		
Construction Material	Stainless steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	433.77	
Heat Duty(Gcal/hr)	1.99021	
Purchase Cost:	$24,229.07	
Bare Module Cost:	$76,806.16	

Heat Exchanger: F2-HX4		
Block Type:	Shell and Tube Heat Exchanger	
Function:	Heat Integration	
Tube:	Inlet	Outlet
Stream	STEAM3	8
Temperature(Celcius)	138.32	130.022
Pressure(bar)	3.43918	3.43918
Shell:	Inlet	Outlet
Stream	7	9
Temperature(Celcius)	112.682	120.022
Pressure(bar)	0.01	0.01
Operating Conditions:		
Tube Flow Rate (kg/hr)	540	
Shell Flow Rate (kg/hr)	56154.718	
Design Data:		
Construction Material	Stainless steel	
Flow Direction	Countercurrent	
Transfer Area(ft^2)	192.27	
Heat Duty(Gcal/hr)	0.283541	
Purchase Cost:	$21,454.28	
Bare Module Cost:	$68,010.05	

Distillation Tower: D1			
Block Type:	Packed Distillation Column		
Function:	Isolates desired product (DPC)		
Materials:	Inlet	Distillate	Bottoms
Stream	S11	S12	S19
Phase	Vapor	Vapor	Liquid
Mass Flow (lb/Hr)	120.56	109.64	2339.65
Volumetric Flow (ft3/Hr)	6531.2	4191.57	34.4
Temperature (°C)	264.73	128.15	206.68
Breakdown(lb/Hr):			
Phenol	641.82	641.41	0.41
Water	1104.8	1104.81	0
DPC	3815.12	1475.88	2339.24
CO	969.46	969.46	0
O_2	0	0	0
Catalyst Mix	0	0	0
Operating Conditions:			
Condenser Pressure (bar)	0.03		
Condenser Temperature (°C)	88.305		
Reboiler Pressure (bar)	0.07		
Reboiler Temperature (°C)	206.6		
Reflux Ratio (molar)	0.651		
Design Data:			
Construction Material	Carbon Steel	Tray Efficiency	N/A
Weight (lbs)	110717	Number of Trays	N/A
Diameter (ft)	15.58	Feed Stage	N/A
Height (ft)	40	Tray Spacing (ft)	N/A
Purchase Cost:	$894,219.40		
Bare Module Cost:	$3,719,952.70		

Distillation Tower: D2			
Block Type:	Tray Distillation Column		
Function:	Helps remove water		
Materials:	Inlet	Distillate	Bottoms
Stream	S15	H2O	S16
Phase	Liquid	Vapor	Liquid
Mass Flow (lb/Hr)	2185.83	49.81	2136.02
Volumetric Flow (ft3/Hr)	30.65	1370.7	33.07
Temperature (°C)	25.25	99.65	139.266
Breakdown(lb/Hr):			
Phenol	629.95	0.038	629.9
Water	80.12	49.7	30.4
DPC	1475.75	0.05	1475.7
CO	0.009	0.009	0
O_2	0	0	0
Catalyst Mix	0	0	0
Operating Conditions:			
Condenser Pressure (bar)	1.01		
Condenser Temperature (°C)	99.65		
Reboiler Pressure (bar)	1.368		
Reboiler Temperature (°C)	152.4		
Reflux Ratio (molar)	1.024		
Design Data:			
Construction Material	Carbon Steel	Tray Efficiency	0.7
Weight (lbs)	109935.06	Number of Trays	11
Diameter (ft)	6.9	Feed Stage	8
Height (ft)	34	Tray Spacing (ft)	2
Purchase Cost:	$270,627.21		
Bare Module Cost:	$1,125,809.20		

Flash Vessel: F1			
Block Type:	Flash Vessel		
Function:	Separates gasses from liquids		
Materials:	Inlet	Overhead	Bottoms
Stream	S1	S2	S5
Phase	Mixed	Vapor	Liquid
Mass Flow (lb/Hr)	140,950	15,523	125,430
Volumetric Flow (ft3/Hr)	27,947	25,996	1,949.23
Breakdown(lb/Hr):			
Phenol	111,000	91.61	110,910
Water	1,114.70	41.4	1073.3
DPC	12,877	4.11E-4	12,877
CO	15,896	15,390	506.4
O_2	0	0	0
Catalyst Mix	64.64	0	64.64
Operating Conditions:			
Pressure (psia)	145		
Temperature (°C)	80		
Equilibrium	Vapor-Liquid		
Design Data:			
Construction Material	Stainless Steel 316	Diameter (ft)	5.240544478
Weight (lb)		Height (ft)	13.10136119
Volume (ft^3)	282		
Purchase Cost:	$243,707.73		
Bare Module Cost:	$743,308.57		

Flash Vessel: F2			
Block Type:	Flash Vessel		
Function:	Separates Catalyst		
Materials:	Inlet	Overhead	Bottoms
Stream	S6	S10	S7
Phase	Mixed	Vapor	Liquid
Mass Flow (lb/Hr)	125,430	125,200	230.26
Volumetric Flow (ft3/Hr)	5,593,600	68,867,000	3.34
Breakdown(lb/Hr):			
Phenol	110,910	110,870	37.99
Water	1073.3	1,073.3	1.9E-3
DPC	12,877	12,750	127.63
CO	506.4	506.4	3.29E-6
O_2	0	0	0
Catalyst Mix	64.64	0	64.64
Operating Conditions:			
Pressure (psia)	0.145		
Temperature (°C)	120		
Equilibrium	Vapor Liquid		
Design Data:			
Construction Material	Stainless Steel 316	Diameter (ft)	1.063
Weight (lb)	130	Height (ft)	4.59
Volume (ft^3)	4.07		
Purchase Cost:	$25,972.38		
Bare Module Cost:	$103,889.53		

Flash Vessel: F3			
Block Type:	Flash Vessel		
Function:	Removes Water and CO		
Materials:	Inlet	Overhead	Bottoms
Stream	S13	F3TOPS	S14
Phase	Mixed	Vapor	Liquid
Mass Flow (lb/Hr)	112,200	2005.74	111,640
Volumetric Flow (ft3/Hr)	236,540	1,091,400	1,645.28
Breakdown(lb/Hr):			
Phenol	110,620	11.46	110,590
Water	1,073.3	1024.7	1,047.54
DPC	2.45E-13	0.138	0
CO	506.4	969.45	3.28
O_2	0	0	0
Catalyst Mix	0	0	0
Operating Conditions:			
Pressure (psia)	0.483		
Temperature (°C)	25		
Equilibrium	Vapor-Liquid		
Design Data:			
Construction Material	Stainless Steel 316	Diameter (ft)	0.55
Weight (lb)	99.2	Height (ft)	4.02
Volume (ft^3)	0.955		
Purchase Cost:	$14,900		
Bare Module Cost:	$104,300.00		

Compressor: COM1		
Block Type:	Centrifugal Compressor	
Function:	Compresses feed stream to D1	
Materials:	Inlet	Outlet
Stream	S10	S11
Temperature (^{o}C)	120	264.73
Pressure (psia)	0.145	1.45
Design Data:		
Construction Material	Stainless steel	
Efficiency	0.72	
Consumed Power (kW)	200.615	
Power Source	Electricity	
Purchase Cost:	$1,020,941.69	
Bare Module Cost:	$4,371,110.81	

Storage Tank: ST1 (Not shown in Process Flowsheet)	
Block Type:	Storage Tank (Horizontal)
Function:	Stores 7 days of reactant
Materials:	
Chemical	Phenol
Operating Conditions:	
Pressure (psi)	217.55
Temperature (°C)	45
Design Data:	
Construction Material	Incoloy-825
Volume (gal)	288,000
Diameter (ft)	25.38
Length (ft)	76.14
Purchase Cost:	$1,230,568
Bare Module Cost:	$3,753,232

Storage Tank: ST2 (Not shown in Process Flow Sheet)	
Block Type:	Storage Tank (Horizontal)
Function:	Stores 7 days of product
Materials:	
Chemical	DPC
Operating Conditions:	
Pressure (psi)	14.5
Temperature (°C)	100
Design Data:	
Construction Material	Incoloy-825
Volume (gal)	54,974
Diameter (ft)	14.6
Length (ft)	43.83
Purchase Cost:	$525,198
Bare Module Cost:	$1,601,920

Equipment Cost Summary

Equipment Cost Summary

The equipment cost summary on the following page summarizes the equipment cost of each unit in this process. Both the purchase cost and the bare module cost of each unit are included. A bare module factor is used for different types of equipment as referenced from Seider et al., and adjustments are made for difference between the 2012 CE index and the CE index used at the time of the print. The CE Index is provided in Appendix F.

Reference Code	Name	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
R1	Reactor Vessel 1	Fabricated Equipment	$873,645.46	3.05	$2,664,618.64
A1	Agitator for R-1	Process Machinery	$133,300.00	1.5	$199,950.00
ST1	Steam Turbine Motor for R-1	Process Machinery	$260,255.28	1	$260,255.28
HC1	Cooling Coils for R-1	Fabricated Equipment	$87,364.55	1	$87,364.55
F1	Flash Column 1	Fabricated Equipment	$243,707.73	3.05	$743,308.57
F2	Flash Column 2	Fabricated Equipment	$25,972.38	4	$103,889.53
D1	Distillation Column 1	Fabricated Equipment	$894,219.40	4.16	$3,719,952.70
D1 Condenser	D-1 Tower Condenser	Fabricated Equipment	$9,200.00	3.17	$57,400.00
D1 Reboiler	D-1 Tower Reboiler	Fabricated Equipment	$19,000.00	3.17	$76,300.00
D1 Reboiler Pump	D-1 Reboiler Pump	Process Machinery	$26,589.31	3.3	$87,744.73
D1 Reboiler Motor	D-1 Reboiler Motor	Process Machinery	$71,677.44	3.3	$236,535.55
D1 Accumulator	D-1 Reflux Accumulator	Fabricated Equipment	$14,500.00	3.05	$102,100.00
D1 Reflux Pump	D-1 Reflux Pump and Motor	Process Machinery	$5,598.60	3.3	$27,400.00
F3	Flash Column 3	Fabricated Equipment	$14,900.00	4	$104,300.00
C2	Condenser 2	Fabricated Equipment	$37,948.50	3.17	$121,571.12
VAC1	Liquid-Ring Pump 1	Process Machinery	$47,680.18	1	$47,680.18
D2	Distillation Column 2	Fabricated Equipment	$270,627.21	4.16	$1,125,809.20
D2 Condenser	D-2 Tower Condenser	Fabricated Equipment	$7,500.00	3.17	$43,800.00
D2 Reboiler	D-2 Tower Reboiler	Fabricated Equipment	$10,700.00	3.17	$59,600.00
D2 Reboiler Pump	D-2 Reboiler Pump	Process Machinery	$7,839.70	3.3	$25,871.01
D2 Reboiler Motor	D-2 Reboiler Motor	Process Machinery	$7,027.20	3.3	$23,189.76
D2 Accumulator	D-2 Reflux Accumulator	Fabricated Equipment	$14,500.00	3.05	$101,400.00
D2 Reflux Pump	D-2 Reflux Pump and Motor	Process Machinery	$4,200.00	3.3	$26,000.00
C1	Condenser 1	Fabricated Equipment	$38,350.51	3.17	$124,002.54
COMP1	Compressor 1	Fabricated Equipment	$1,020,941.69	2.15	$4,371,110.81
C3	Condenser 3	Fabricated Equipment	$18,245.85	3.17	$70,305.77
C4	Condenser 4	Fabricated Equipment	$24,523.05	3.17	$91,235.62
F2-HX1	Heat Exchanger 1	Fabricated Equipment	$61,419.64	3.17	$194,700.25
F2-HX2	Heat Exchanger 2	Fabricated Equipment	$22,400.02	3.17	$71,008.06
F2-HX3	Heat Exchanger 3	Fabricated Equipment	$24,229.07	3.17	$76,806.16
F2-HX4	Heat Exchanger 4	Fabricated Equipment	$21,454.28	3.17	$68,010.05
F4	Flash Column 4	Fabricated Equipment	$11,998.94	4	$47,995.78
P1	Pump 1	Process Machinery	$3,478.52	3.3	$11,479.12
EM1	Electric Motor for P-1	Process Machinery	$3,162.24	3.3	$10,435.39
P2	Pump 2	Process Machinery	$4,905.89	3.3	$16,189.43
EM2	Electric Motor for P-2	Process Machinery	$1,054.08	3.3	$3,478.46
P3	Pump 3	Process Machinery	$3,683.01	3.3	$12,153.95
EM3	Electric Motor for P-3	Process Machinery	$527.04	3.3	$1,739.23
P4	Pump 4	Process Machinery	$3,165.72	3.3	$15,967.59
EM4	Electric Motor for P-4	Process Machinery	$756.43	3.3	$2,496.22
ST1	Storage Tank 1 (Phenol)	Storage	$1,230,568.07	3.05	$3,753,232.61
ST2	Storage Tank 2 (DPC)	Storage	$525,219.88	3.05	$1,601,920.65
SPT1	Pump, Valve, Mixer & Splitter	Spares			$1,925,619.67
SH1	Shipping Loading Spots	Miscellaneous			$1,200,000.00
	Total				$20,590,308.50

Fixed-Capital Investment Summary

Fixed-Capital Investment Summary

The fixed costs for DPC production are comprised of equipment and shipping costs as shown in the previous section. The bare module factor includes the direct and indirect costs for each module: the material, fabrication and installation costs. However, additional costs exist, including site preparation and the costs of land and of labor. Because this plant complex will be built in the Gulf Coast, which already has a highly integrated distribution network, only 6% of the total bare module costs are allocated for site preparations. An additional 5% of the total bare module costs are allocated for the service facilities necessary for a plant of this scope, as recommended by Seider, *et al*. This includes costs for utility lines, control rooms, onsite laboratories for feed and product testing, maintenance shops, and other necessary buildings. No utility-related facilities are included in this investment scope, since utilities will be purchased from local vendors.

This process involves few very hazardous materials or volatile components; contingencies can be projected at a moderate industry standard 7% of direct permanent investment. Another 3% of the direct permanent investment is recommended to account for contractor fees, as estimated by Guthrie (1969). This plant will not require a remarkably large footprint, so the cost of land is predicted to be only 2.5% of total depreciable capital. In addition, the startup costs should not be highly prohibitive because this process is fairly standard in the scope of its design, with the exception of a vacuum system. Therefore, a small margin is tacked on to the 2% recommendation offered by Seider, et al. A summary of the total permanent investments is given in Table XVII.

Table XVII: *Total permanent investment input assumptions*

Investment Considerations	Cost	Basis
Cost of Site Preparations	6.0%	of Total Bare Module Cost
Cost of Service Facilities	5.0%	of Total Bare Module Cost
Utility plants and related Facilities	0.0%	
Contingencies Cost	7.0%	of Direct Permanent Investment
Contractor Fees	3.0%	of Direct Permanent Investment
Cost of Land	2.0%	of Total Bare Module Cost
Cost of Royalties	0.0%	
Cost of Plant Start-Up	4.0%	of Total Bare Module Cost

To calculate the full capital investment, the bare module costs are added to all aspects of the direct permanent investment, the total depreciable capital, and the total permanent investments. Spare parts are to be kept on hand for pumps, valves, splitters, and mixers to minimize the plant downtime in the event of a pump failure. Additional spare parts are cost-prohibitive to keep in inventory and will be managed on an "as needed" basis during the plant's operation. An additional consideration is the inclusion of a shipping cost associated with loading spots required for the unloading of raw material, and the loading for distribution of DPC. An estimated value was based on recommendations from the industrial consultants. The full capital investment is calculated in Table XVIII on the following page.

***Table XVIII**: Fixed Capital Investment Summary*

Investment Summary	
Bare Module Costs	
Fabricated Equipment	$14,226,589.35
Process Machinery	$1,008,565.90
Spares	$1,925,619.67
Storage	$5,355,153.26
Other Equipment	$1,200,000.00
Total	$23,715,928.18
Direct Permanent Investment	
Cost of Site Preparation	$1,422,955.69
Cost of Service Facilities	$1,185,796.41
Costs for Utility Plants	0
Total	$26,324,680.28
Depreciable Capital	
Cost of Contingencies	$1,842,727.62
Contractor Fees	$789,740.41
Total	$28,957,148.31
Total Permanent Investment	
Cost of Land	$474,318.56
Cost of Start-Up	$948,637.13
Cost of Royalties	0
Total - Raw	$30,380,104.00
Size Factor	1
Total Adjusted Investment	$30,380,104.00

Operating Cost and Economic Analysis

Economic Assumptions and Project Operations

It is assumed that the construction period will take a total of two years and that production will begin to ramp up starting in 2016. The permanent investment will be split for the two years of construction. The cost of DPC will increase by 1% each year after production to account for inflation.

***Table XIX**: Project assumptions and operations summary*

General Information

Process Title:	*Phosgene-Free Route to Diphenyl Carbonate*
Product:	*Diphenyl Carbonate (DPC)*
Plant Site Location:	*Gulf Coast*
Size Factor:	*1*
Operating Hours per Year:	*8620*
Operating Days Per Year:	*360*
Operating Factor:	*0.9863*

Product Information:

Yield*:*

12,749.6	lb of DPC per hour
305,281.2	lb of DPC per day
109,901,241.7	lb of DPC per year

Price: *$1.75 per lb*

Table XIX (continued): *Project assumptions and operations summary*

Operational Ramp Up Schedule

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation	DPC Price
2013	Design		0.0%	*5 year MARCS*	*per lbs.*
2014	Construction	50%	0.0%		
2015	Construction	50%	0.0%		
2016	Production	0%	41.0%	20.00%	$1.75
2017	Production	0%	67.5%	32.00%	$1.79
2018	Production	0%	90.0%	19.20%	$1.82
2019	Production	0%	90.0%	11.52%	$1.86
2020	Production	0%	90.0%	11.52%	$1.89
2021	Production	0%	90.0%	5.76%	$1.93
2022	Production	0%	90.0%		$1.97
2023	Production	0%	90.0%		$2.01
2024	Production	0%	90.0%		$2.05
2025	Production	0%	90.0%		$2.09
2026	Production	0%	90.0%		$2.13
2027	Production	0%	90.0%		$2.18
2028	Production	0%	90.0%		$2.22
2029	Production	0%	90.0%		$2.26
2030	Production	0%	90.0%		$2.31

Operating Cost Summary

Variable Costs

Variable costs are broken down into several major categories: raw material pricing of catalysts and other reactants, utility costs, labor costs, and other general expenses that are incurred with the operation of a commodity-scale production facility. The problem statement, found in the Appendix, provided long-term average prices for the following components: phenol, carbon monoxide, and oxygen. Bulk catalyst prices are difficult to obtain since purchasing information is commonly given at laboratory scale price points. Based on the recommendation of the industrial consultants, a discounted bulk laboratory rate for the palladium and organic catalysts was estimated. The price of the catalyst mix is a weighted average price of the component catalysts for the proportion in which they are used. Further considerations on the topic of catalyst pricing, including sensitivity analysis, can be found later in this report. To prevent depletion of catalytic activity, the catalyst slurry will be replenished every six months. The raw material costs for this DPC production process are summarized in Table XX.

Table XX: *Raw materials cost for continuous operation*

Material	lb/hr	lb/yr	$/lb	$/yr
PHENOL	11502.46	99151179	0.7	$ 69,405,825.54
CO	2944.678	25383124	0.15	$ 3,807,468.65
O2	952.361	8209352	0.03	$ 246,280.55
CATALYST MIX	0.646	5568.52	12276.47	$ 68,361,771.86
TOTAL				$ 141,821,346.60

Utility costs include the costs of steam, cooling water, and electricity. Steam is being used at pressures of 50 and 300 psi, and prices for steam are taken from Seider, et al. and are adjusted to 2013 dollar amounts by taking inflation into consideration ("Inflation Calculator"). Detailed utility cost calculations are provided in *Table XXXIII* and *Table XXXIV* in Appendix H, and the final numbers are included in Table XXI.

Labor costs and general expenses include selling and transfer expenses, research expenses, administrative expenses, plant operator expenses, and managerial compensation. Staring with an estimate of general expenses accounting for 10.5% of total sales, a breakdown of general expenses is shown in Table XXI. Bearing in mind the relevance of technological development to the field we will be operating in, it is reasonable to allocate the majority of general expenses to a direct and allocated research budget.

Table XXI: *Complete Variable Cost Summary*

Variable Cost Summary				
Note: All Costs at 100% Capacity				
General Expenses				
				$/yr
	Selling & Transfer Expenses			$4,593,750.00
	Direct Research			$6,431,250.00
	Allocated Research			$1,470,000.00
	Administrative Expense			$2,205,000.00
	Management Incentive Compensation			$3,675,000.00
	Total General Expenses			$18,375,000.00
Raw Materials				
		lb/hr	lb/yr	$/lb	
	Phenol	11502.46	99151179	0.7	$69,405,825.54
	Carbon Monoxide	2944.678	25383124	0.15	$3,807,468.65
	Oxygen	952.361	8209352	0.03	$246,280.55
	Catalysts	0.646	5568.52	12276.47	$68,361,771.86
	Total Material Cost				$141,821,346.60
Utilities				
	Steam				$1,334,149.47
	Cooling Water				$54,874.35
	Electricity				$1,048,479.41
	Total Utilities Cost				$2,437,503.23
Total Variable Costs:					$162,633,849.83

Table XXI shows that variable costs represent 84.56%, or $162,633,849.83, of the hypothetical sales at full production capacity, or $192,327,172.98. In other words, $1.48 of variable costs is incurred for every pound of DPC sold, which leaves a profit margin of $0.27 per pound of DPC sold. Figure 11, shown as exploded pie charts on the following page, shows a breakdown of the total variable costs.

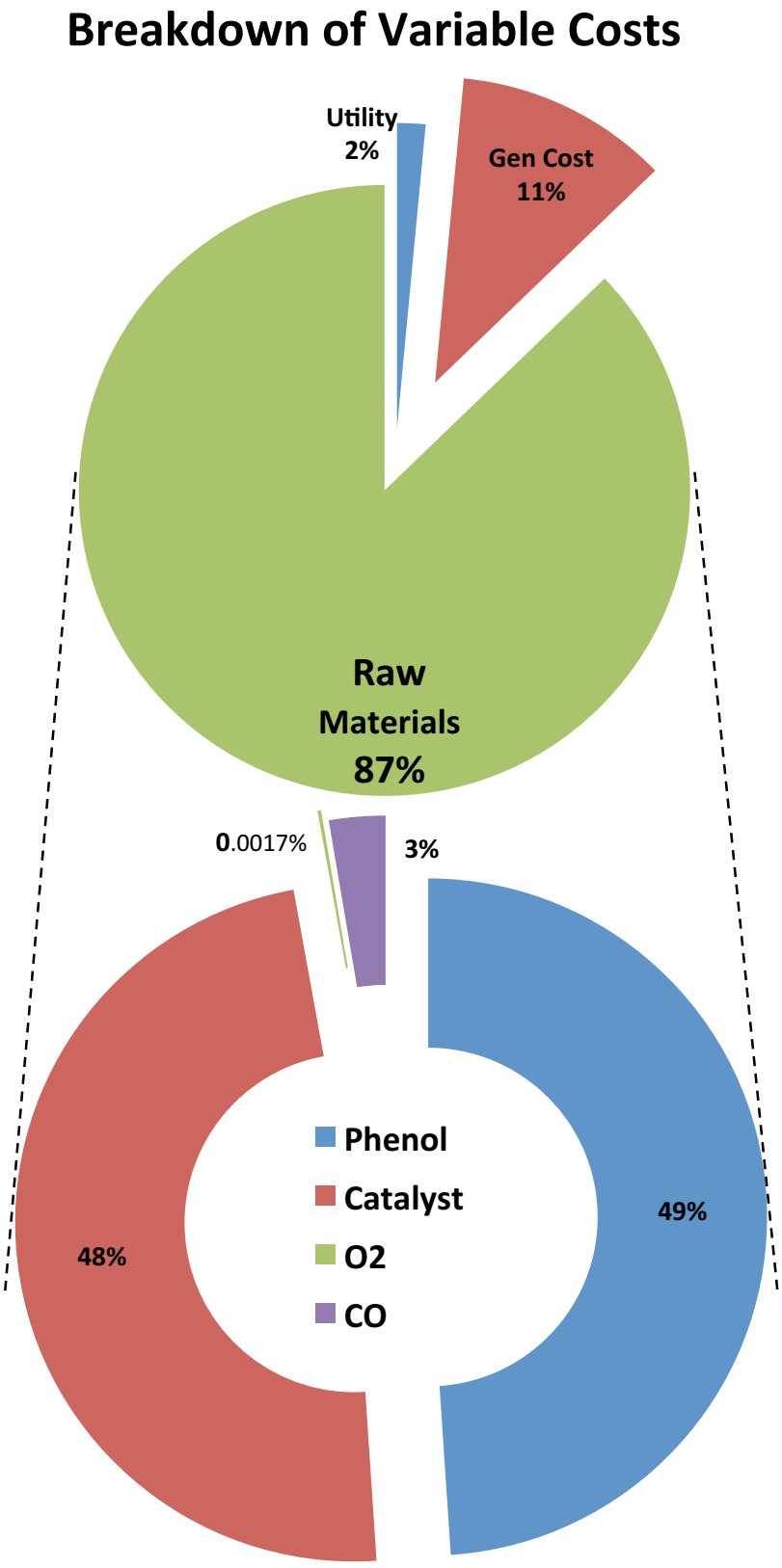


Figure 11: *Breakdown of Variable Costs*

Fixed Costs

Since fixed costs are not dependent on the amount of DPC produced, they are shown separately in Table XXII on the following page. The plant operator costs along with annual maintenance, operating overhead and property taxes and insurance are illustrated below. These fixed costs are trivial in comparison to the variable costs and are therefore not heavily considered when determining the overall profitability of the project.

Table XXII: *Fixed cost summary*

Process Sections:
1. Feed Handling 2. Reactor System 3. Vacuum System 4. Product Purification 5. Recycle System

Operations:	Note: *2 per shift,5 shifts, 40hr/week, 52 week/yr*
	Cost / yr
Direct Wages & Benefits, DWB = (operators/shift)*(Shifts) x (2080 hr/yr)($/hr)	$728,000.00
Direct Salaries & Benefits = .15 (DWB)	$109,200.00
Operating Supplies & Services = 0.06 (DWB)	$43,680.00
Technical Assistance to Manufacturing = 60,000 (Shifts)	$300,000.00
Control Lab = 65,000 (Shifts)	$325,000.00
Total Labor Operating Cost, O:	$1,505,880.00
Maintenance	C_{TDC} = *$30,380,104.00*
Wages & Benefits, MWB = 3.5% of C_{TDC}	$1,063,303.64
Salaries & Benefits = 25% of MWB	$265,825.91
Materials & Services = 100% of MWB	$1,063,303.64
Maintenance Overhead = 5% of MWB	$53,165.18
Total Maintenance Cost, M:	$2,445,598.37
Operating Overhead	
22.8% of M&O-SW&B*:	$493,923.14
Property Taxes & Insurance	
2 % of C_{TDC}:	$607,602.08
Total Fixed Costs:	$5,053,003.59

Cash Flow and Profitability Analysis

Project Economics

The following metrics were used to determine the feasibility and overall profitability of the base case design: net present value analysis (NPV), internal rate of return (IRR), return on investment (ROI), and payback period (PP). The NPV was calculated using a 15% discount rate, which is recommended by Seider, *et al*, and negative numbers are represented by parentheses. A 2% general inflation rate was used for the base case profitability and cash flow analysis. Further considerations on top of the base case will be described after an initial feasibility and profitability analysis, which is presented in the tables on the following pages.

***Table XXIII**: Cash flow summary*

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Taxable Income	Taxes	Net Earnings	Cash Flow	Cumulative NPV @ 15%
2013	0%		-	-	-	-	-	-	-	-	-	-	-
2014	0%		-	(14,579,700)	-	-	-	-	-	-	-	(14,579,700)	(12,678,000
2015	0%		-	(14,579,700)	(7,398,400)	-	-	-	-	-	-	(21,978,100)	(25,264,900
2016	41%	$1.75	77,892,500	-	(4,521,300)	(8,996,600)	(4,286,000)	(5,501,800)	59,108,100	(21,870,000)	37,238,100	38,218,600	(23,090,800
2017	65%	$1.79	128,003,300	-	(4,521,300)	(14,784,400)	(4,371,800)	(8,802,900)	100,044,400	(37,016,400)	63,027,900	67,309,500	(17,010,500
2018	90%	$1.82	180,087,500	-	-	(20,800,100)	(4,459,200)	(5,281,700)	149,546,500	(55,332,200)	94,214,300	99,496,000	(8,598,600)
2019	90%	$1.86	183,689,200	-	-	(21,216,100)	(4,548,400)	(3,169,000)	154,755,700	(57,259,600)	97,496,100	100,665,100	(1,078,800)
2020	90%	$1.89	187,363,000	-	-	(21,640,400)	(4,639,300)	(3,169,000)	157,914,200	(58,428,300)	99,486,000	102,655,000	5,945,400
2021	90%	$1.93	191,110,300	-	-	(22,073,200)	(4,732,100)	(1,584,500)	162,720,400	(60,206,500)	102,513,800	104,098,400	12,295,300
2022	90%	$1.97	194,932,500	-	-	(22,514,700)	(4,826,800)	-	167,591,000	(62,008,700)	105,582,300	105,582,300	18,037,600
2023	90%	$2.01	198,831,100	-	-	(22,965,000)	(4,923,300)	-	170,942,800	(63,248,800)	107,694,000	107,694,000	23,376,900
2024	90%	$2.05	202,807,700	-	-	(23,424,300)	(5,021,800)	-	174,361,700	(64,513,800)	109,847,900	109,847,900	28,328,800
2025	90%	$2.09	206,863,900	-	-	(23,892,800)	(5,122,200)	-	177,848,900	(65,804,100)	112,044,800	112,044,800	32,910,700
2026	90%	$2.13	211,001,200	-	-	(24,370,600)	(5,224,700)	-	181,405,900	(67,120,200)	114,285,700	114,285,700	37,141,400
2027	90%	$2.18	215,221,200	-	-	(24,858,000)	(5,329,100)	-	185,034,000	(68,462,600)	116,571,400	116,571,400	41,040,300
2028	90%	$2.22	219,525,600	-	-	(25,355,200)	(5,435,700)	-	188,734,700	(69,831,800)	118,902,900	118,902,900	44,627,000
2029	90%	$2.26	223,916,100	(25,862,300)	-	(25,862,300)	(5,544,400)	-	192,509,400	(71,228,500)	121,280,900	121,280,900	47,921,300
2030	90%	$2.31	228,394,500	-	-	(26,379,600)	(5,655,300)	-	196,359,600	(72,653,000)	123,706,500	140,147,400	51,560,200

***Table XXIV**: Profitability measures and sensitivity analyses*

Profitability Measures

The Internal Rate of Return (IRR) for this project is **36.10%**

The Net Present Value (NPV) of this project in 2013 is **$ 51,560,200**

ROI Analysis (Third Production Year)

Annual Sales	**180,087,472**
Annual Costs	**(156,333,452)**
Depreciation	**(2,332,756)**
Income Tax	**(7,925,868)**
Net Earnings	**13,495,396**
Total Capital Investment	**35,808,862**
ROI	**37.69%**

Sensitivity Analyses

Effect of variable cost fluctuation

		Variable Costs									
	$11,106,894	$13,328,273	$15,549,652	$17,771,031	$19,992,410	***$22,213,788***	$24,435,167	$26,656,546	$28,877,925	$31,099,304	$33,320,683
$0.88	22.23%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.05	42.41%	25.77%	2.12%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.23	57.58%	44.34%	28.81%	8.71%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.40	70.26%	58.84%	46.12%	31.50%	13.56%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.58	81.32%	71.12%	60.03%	47.78%	33.91%	17.49%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.75	91.23%	81.91%	71.94%	61.16%	49.33%	36.10%	20.83%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.93	100.25%	91.62%	82.48%	72.73%	62.23%	50.78%	38.11%	23.76%	6.73%	Negative IRR	Negative IRR
$2.10	108.57%	100.49%	92.01%	83.03%	73.49%	63.25%	52.15%	39.97%	26.38%	10.77%	Negative IRR
$2.28	116.31%	108.69%	100.73%	92.38%	83.57%	74.22%	64.22%	53.45%	41.70%	28.75%	14.21%
$2.45	123.57%	116.34%	108.81%	100.96%	92.74%	84.08%	74.92%	65.15%	54.67%	43.33%	30.93%
$2.63	130.41%	123.51%	116.36%	108.93%	101.19%	93.09%	84.58%	75.59%	66.04%	55.84%	44.85%

Product Price

This sensitivity analysis on the variable cost is significant because utility costs and raw material costs are likely to increase throughout the duration of this plant's lifetime. The base case proves itself to be a viable option be demonstrating returns. Positive IRR values despite increasing variable costs indicate that this project is economically viable throughout a range of conditions and in the long term.

Further Sensitivity Analysis

Several factors have the ability to significantly modify the profitability of this process either positively or negatively, and it would be remiss to exclude the implications of DPC product price and catalyst price.

The base case for DPC production assumes an inflationary adjustment of 2% for each year of sales. Table XXV shows the effect of a range of inflation rates on the NPV; the base case scenario is highlighted.

***Table XXV**: The effect of inflation rate on product price*

		Product Price Inflation Rate						
		0.0%	**0.5%**	**1.0%**	**1.5%**	**2.0%**	**2.5%**	**3.0%**
Product Price	**$1.30**	-$89,009,800	-$80,755,400	-$72,208,100	-$65,938,800	-$63,356,600	-$56,805,300	-$47,343,600
	$1.40	-$68,188,600	-$59,299,300	-$50,094,600	-$42,439,000	-$40,562,200	-$32,575,100	-$22,356,400
	$1.50	-$47,367,400	-$37,843,200	-$27,981,100	-$18,939,200	-$17,767,800	-$8,344,900	$2,630,800
	$1.60	-$26,546,200	-$16,387,100	-$5,867,600	$4,560,600	$5,026,600	$15,885,300	$27,618,000
	$1.70	-$5,725,000	$5,069,000	$16,245,900	$27,821,000	$28,060,400	$40,115,500	$52,605,200
	$1.75	$4,685,600	$15,797,050	$27,302,650	$39,218,200	$51,560,200	$64,345,700	$77,592,400
	$1.80	$15,096,200	$26,525,100	$38,359,400	$50,615,400	$75,060,000	$76,460,800	$90,086,000
	$1.90	$35,917,400	$47,981,200	$60,472,900	$73,409,800	$98,559,800	$100,691,000	$115,073,200
	$2.00	$56,738,600	$69,437,300	$82,586,400	$96,204,200	$122,059,600	$124,921,200	$140,060,400
	$2.10	$77,559,800	$90,893,400	$104,699,900	$118,998,600	$145,559,400	$149,151,400	$165,047,600

The NPV remains positive for a wide range of inflation rates. Therefore, the profitability of this process is sufficiently positive to accommodate for price and interest rate fluctuations.

Table XXVI illustrates the calculation of the weighted average price of the catalyst mixture. The organic co-catalyst (ligand) is 3,6-diaminocarbazole, the base catalyst is sodium hydroxide, the reduction-oxidation catalyst is $Mn(acac)_2$ and the phase transfer catalyst is $[^nBu_4N]I$.

Table XXVI: *Weighted average cost of catalyst mix*

	Catalysts				
	PdCl2	Organic	Base	Redox	Phase
Ratios	1	1	2	1	1
MW (g/mol)	177.33	325	40	253.154	369.37
Amount In MIX	177.33	325	80	253.154	369.37
% By mass	0.1471797	0.269742	0.066398	0.210112	0.306568
Individual Cost ($/g)	15	10	0.05	0.86	0.426
Aporte ($/g)	2.2076949	4.35364	0.00332	0.180696	0.130598
Weighted Average Cost for MIX		**Continuous Feed**		**Total Cost per Year**	
12276.47	($/lbs)	5568.52	(lb/yr)	68361768.72	$/yr

Palladium chloride and the organic co-catalyst drive the overall price of the catalytic mixture, and a sensitivity analysis was performed to determine the effect of variations in their prices. In the first catalyst sensitivity analysis, the price of the organic co-catalyst was reduced to $5/g from $10/g, and in the second catalyst sensitivity analysis, the price of the palladium catalyst was reduced to $10/g from $15/g.

Table XXVII: *Catalyst price variation with change in organic catalyst price*

	PdCl2	Organic	Base	Redox	Phase
Individual Cost ($/g)	15	5	0.05	0.86	0.426
Aporte ($/g)	2.2076949	1.34871	0.00332	0.180696	0.130598
Weighted Average Cost for MIX		**Continuous Feed**		**Total Cost per Year**	
8516.24	($/lbs)	5568.52	(lb/yr)	47422876	$/yr
		Difference In Cost:		**$20,938,893**	

A variable cost savings of $20,939,893 is significant and would change the profitability margin from 27 cents to 46 cents per pound of DPC sold. This represents a 41.3% increase in profitability based on variable costs alone. The following table considers the impact of a decrease in price of the palladium chloride catalyst in addition to change in price of the organic co-catalyst.

Table XXVIII: *Catalyst price variation with change in palladium and organic catalyst prices*

	PdCl2	Organic	Base	Redox	Phase
Individual Cost ($/g)	10	5	0.05	0.86	0.426
Aporte ($/g)	2.2076949	1.34871	0.00332	0.180696	0.130598
Weighted Average Cost for MIX		**Continuous Feed**		**Total Cost per Year**	
6837.27	($/lbs)	5568.52	(lb/yr)	38,407,575	$/yr
		Difference In Cost:		**$29,954,194**	

A variable cost savings of $29,954,194 would increase the profitability per pound of DPC sold to 54 cents. This represents a 50.3% increase in profitability based solely on variable cost considerations, and it is apparent that the catalyst pricing has a large impact on overall profitability. If the catalyst costs were to increase, it might be more economical to purchase the raw materials and synthesize the

necessary catalysts in-house. However, such a process is outside the scope of this design report and must be left to the acquirers of this design.

Additional Considerations

Additional Considerations

Environmental Concerns

In light of the fact that the motivation for this project is largely out of environmental and safety concerns, the effects of this process on the environment must be carefully evaluated. When this process is held against the United States Environmental Protection Agency's (EPA) twelve principles of green chemistry, developed in 2006, it is clear that this process is quite environmentally sustainable:

1. It is better to prevent waste than to treat or clean up waste after it is formed.

The highlight of this process is that the only major byproduct of the process is water. This is in stark contrast to the phosgene-based process in which a stoichiometric amount of sodium chloride is formed in the process. Sodium chloride is a waste chemical that must be properly removed and disposed of.

2. Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

All of the materials used in the process are incorporated in the product, with water as the only byproduct of the reaction. Therefore this phosgene-free synthesis of diphenyl carbonate is highly atom economical.

3. Wherever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

Phenol must be handled with care since it can cause chemical burns, and carbon monoxide is acutely toxic for humans if inhaled. Although the synthetic methodology of this process could not avoid using toxic reagents, the need to use stoichiometric amounts of phosgene was eliminated.

4. Chemical products should be designed to preserve efficacy of function while reducing toxicity.

A different route to diphenyl carbonate was designed, and the product design was untouched.

5. The use of auxiliary substances (e.g. solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used.

Another highlight of this process is that no solvents or separating agents were used in any of the process equipment. The reaction is run neatly in molten phenol, and the separation of DPC is accomplished via vacuum distillation.

6. Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure.

The reactor operates under relatively low temperatures, but the reactor must be maintained at 10 bar or above to keep a practically reasonable conversion and selectivity. This stands in contrast to the phosgene process, where the reaction is carried out around ambient temperature and pressure due to the high reactivity of phosgene.

The separation train requires the use of pressurized steam to achieve a high temperature for the distillation of diphenyl carbonate from phenol. The energy requirement to maintain a partial vacuum also increases the energy input of this design. Again, this stands in contrast to the phosgene process, where the isolation of diphenyl carbonate is relatively easy and requires a small energy input.

7. A raw material or feedstock should be renewable rather than depleting wherever technically and economically practicable.

Both phenol and carbon monoxide are derived from petroleum; phosgene is produced from carbon monoxide and chlorine. Finding an alternative, renewable feedstock is an ongoing challenge for the chemical industry.

8. Reduce derivatives - Unnecessary derivatization (blocking group, protection/ deprotection, temporary modification) should be avoided whenever possible.

In the phosgene route to the production of diphenyl carbonate, a stoichiometric amount of base, namely sodium hydroxide, must be used to convert phenol to sodium phenolate. This step does not appear in this proposed process, and only a substoichiometric amount of sodium hydroxide is necessary to turn over the catalytic cycle.

9. Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

The palladium-catalyzed oxidative carbonylation of phenol is over 99% selective for diphenyl carbonate in the presence of carbazole, which serves as the organic ligand. This efficiency is in stark contrast to the phosgene route to the production of diphenyl carbonate, since phosgene must be used in stoichiometric amounts.

10. Chemical products should be designed so that at the end of their function they do not persist in the environment and break down into innocuous degradation products.

Hydrolysis of diphenyl carbonate results in the formation of carbon dioxide and phenol.

11. Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.

12. Substances and the form of a substance used in a chemical process should be chosen to minimize potential for chemical accidents, including releases, explosions, and fires.

Phosgene is a hazardous gas that needs to be handled with extreme care to prevent releases. Although carbon monoxide poses a similar threat, phenol represents a smaller chemical hazard and conventional handling of chemicals is required.

Palladium Chloride Catalyst

Palladium is categorized as a platinum group metal (PGM) and, as part of the ore mining industry, is still rebounding from the recession as reflected by industry growth and increasing prices. Therefore, the volatility of the cost of palladium chloride is important to monitor when considering the long-term economics of this project.

Demand for platinum and palladium is increasing largely as a function of the increasing global transportation market, since a main end product of these metals is catalytic convertors used in vehicles. Automobile manufacturing is such a dominant driver of the platinum and palladium market that lowered production of catalytic converters in 2012 corresponded with a 6.9% decrease in price ("Products and Markets", IBISWorld). This trend is expected to reverse in 2013 and in future years with a burgeoning middle class in the Far East, particularly in China and India, that will create an increasing demand for cars and trucks. Therefore, a rebounding price in international markets could affect the current pricing quotes for $PdCl_2$ as the cost of synthesizing palladium chloride increases. This market volatility is reflected in the risk analysis portion of this report.

The DPC production process described in this report requires a catalyst mixture comprised of palladium chloride, sodium hydroxide, $Mn(acac)_2$, $[^nBu_4N]I$, and 3,6-diaminocarbazole. While a detailed calculation of the total catalyst pricing was discussed earlier in this report, the most economically

volatile component is palladium chloride, and that component was used as the basis of the market research pertaining to the catalyst mixture.

Organic Catalyst Cost

One major factor in this project's operating cost is the price of the catalysts. The price of the organic catalyst, 3,6-diaminocarbazole, was found to be significantly higher than those of the other catalysts needed and significantly higher than those of chemically comparable catalysts. US Patent 8,212,066, on which this project is based, cites 3,6-diaminocarbazole as the best organic co-catalyst to use for this process but uses a similar compound, 3,6-dibromocarbazole, in the experiments. Since the chemistry of the two co-catalysts is very similar in this case, it is possible that the cost of 3,6-diaminocarbazole was prohibitive. Should that be the case, the cost of 3,6-diaminocarbazole would be extremely prohibitive at an industrial scale. Two more economically feasible alternatives could be considered: using a less expensive catalyst, or creating the compound in-house with the help of a chemist. To determine the cost of the catalyst in this report, an estimated cost of similar catalysts was used; when building this plant, each of the above options should be thoroughly analyzed.

Startup

Although a relatively small amount of fresh feed is needed because the recycle streams in this process contain almost all of their target components, the initial charge requires a large amount of feed. The fresh feed to the continuously-operating process contains only 9.5% as much phenol, 20% as much CO, and 1% as much catalyst mixture as the startup feed does. The continuously fed feed and the startup feed, however, contain the same amount of oxygen, since oxygen is the limiting reactant and is assumed to be entirely consumed. The initial charge incurs such an exorbitant cost in raw materials that

a gradual startup or multiple-reactor system are important options to consider when building this plant, and the costs included in this report represent estimates based on continuous operation.

Conclusion and Recommendations

Conclusions and Recommendations

Based on the novel phosgene-free reaction patented in US Patent 8,212,066 and on several assumptions made regarding the reaction chemistry, process equipment, and economic situation, the process for producing DPC via the oxidative carbonylation of phenol presented in this report is a technologically and economically favorable process. This process presents significant advantages over current processes in its simplicity and environmental sustainability, as well as in its economic feasibility.

The process design described in this report is comprised of relatively few and reasonably-sized blocks, making this design attractive and cost-efficient. The recycle loops, which recycle 80-90% of the unreacted carbon monoxide and phenol and 99% of the catalysts, greatly decrease the material costs and reduce the amount of waste chemicals that are deposited into the environment. The heat integration network that takes full advantage of the latent heat in the process streams reduces the need for saturated steam by 96% and the need for cooling water by 68%, which also decreases the variable costs and is environmentally efficient. The net present value of this project was determined to be $51,560,200 with a return on investment of 37.69% and an internal rate of return of 36.1%.

Despite the promising technological and economic features of this process, there are risks and further considerations that must be taken into account before this plant can be built. Further investigation is needed into the reaction mechanism referred to in the patent to increase reaction conversion and find alternate organic co-catalysts that are more economically viable. Higher reaction conversion would decrease the need for and cost of fresh reactants and lead to increased productivity and increased profit margins. A chemically similar yet less expensive organic co-catalyst would have significant results on the economics of this project, and various co-catalyst options should be looked into. Additionally, the price volatility of palladium must be carefully watched to carefully predict the economic success of this project. The main environmental risk in this process is the release of carbon

monoxide into the environment, and ways to safely dispose of it, such as incineration, should be considered.

Although the effects of these risks and other considerations pending analysis are unclear at this stage, the further considerations listed here are able to be easily evaluated. Therefore, based on the technological simplicity, economic feasibility, and environmental sustainability featured in this process, it is recommended to move forward with this proposal and evaluate the risks considered here to develop an even more comprehensive and efficient design for this phosgene-free route to DPC.

Acknowledgements

Acknowledgements

We are incredibly grateful for all of the guidance, advice, and assistance provided by our faculty advisor, professors, and industrial consultants throughout this process. They have given so much of their time and energy to guide us since the beginning of this project and to help us succeed. We would like to thank Professor Leonard Fabiano, Dr. Raymond Gorte, Dr. Warren Seider, Mr. Bruce Vrana, Mr. Richard Bockrath, Mr. John Wismer, Mr. Steven Tieri, and Mr. Adam Brostow for their help on our overall process design, for sharing their ASPEN expertise and helping us troubleshoot our simulations, for providing us with economic heuristics and resources, and for sharing their best practices both from industry and from working with project teams in the past. We would especially like to thank Professor Fabiano for taking many hours out of his schedule to help us develop and troubleshoot our ASPEN simulations and to provide us with guidance on equipment sizing. In addition, we would like to thank Mr. Bruce Vrana, the author of the problem statement, for sharing his industry expertise and guiding us during our process design.

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Appendix

Appendix A: Problem Statement

7. New Phosgene-Free Route to Polycarbonates (recommended by Bruce M. Vrana, DuPont)

Polycarbonates are particularly valued for their optical clarity and impact resistance, and are used in CD, DVD and Blu-ray discs among many other applications. Polycarbonates have historically been made using highly toxic phosgene to make the intermediate diphenyl carbonate (DPC). Besides the hazards of using phosgene, the process must also dispose of byproduct NaCl. Some of the routes to DPC also have troublesome azeotropes. A phosgene-free route to DPC would be more economical and environmentally acceptable.

Your company's chemists have developed a catalyst and co-catalysts for the direct oxidative carbonylation of phenol to DPC. The catalyst is a palladium halide, with nitrogen-containing heterocyclic compounds as the co-catalysts.

Your team has been assembled to develop a plant design to put this new catalyst into operation on the U.S. Gulf Coast. Management desires a plant to produce 100MM lb/yr of DPC. They also desire a plant that uses this technology in the most economical way. You will need to decide on the most economical co-catalyst, based on the performance, cost, and availability of the co-catalyst.

Phenol can be purchased for $0.70/lb. Oxygen can be purchased for $0.03/lb at 500 psig. Carbon monoxide can be purchased for $0.15/lb at 500 psig. DPC can be sold for $1.75/lb. All prices are forecasts by your marketing organization for long-term average prices, expressed in 2013 dollars for the quantities needed delivered to your site or sold from your site.

You will need to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before approving an expensive pilot plant to provide the scale-up data you need to complete the design. Test your economics to reasonable ranges of your assumptions. If there are any possible "show-stoppers" (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

The plant design should be as environmentally friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Remember that, if the plant is approved, you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference

U.S. Patent 8,212,066, July 3, 2012, assigned to China Petrochemical Development Corp.

Appendix B: US Patent 8,212,066: Process for Producing Diaryl Carbonates

United States Patent 8,212,066
Huang , et al. July 3, 2012

Process for producing diaryl carbonates

Abstract
The present invention relates to a process for producing diaryl carbonates, which is to synthesize diaryl carbonates by oxidative carbonylation of phenols with carbon monoxide and oxygen, and in particular, to synthesize diphenyl carbonate from phenol. The present invention is characterized in that a catalytic system comprising a metal halide catalyst and one or more co-catalysts of nitrogenous heterocyclic compounds is used to increase the convertibility, selectivity and yield of this catalytic reaction.

Inventors: Huang; Zhen Wei (Chiayi, TW), Chang; Chih Wei (Ta-Sheh, TW), Tsai; Chia Jung (Kaohsiung, TW)
Assignee: China Petrochemical Development Corporation (Taipei, TW)
Family ID: 44152010
Appl. No.: 12/813,185
Filed: June 10, 2010

Foreign Application Priority Data

Dec 21, 2009 [TW] 98143851 A

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Current International Class: C07C 68/00 (20060101)
Current CPC Class: C07C 68/005 (20130101); C07C 68/005 (20130101); C07C 69/96 (20130101)
Field of Search: 558/260,270,274

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Primary Examiner: Shameem; Golam M M
Attorney, Agent or Firm: Sughrue Mion, PLLC

Claims

What is claimed is:

1. A process for producing a diaryl carbonate, in which the diaryl carbonate is synthesized by oxidative carbonylation of a phenol with carbon monoxide and oxygen, characterized in that a catalytic system comprising a metal halide catalyst and one or more co-catalysts of nitrogenous heterocyclic compounds is used.

2. The process according to claim 1, wherein the metal halide catalyst is a palladium halide.

3. The process according to claim 1 or 2, wherein the co-catalyst is one or more nitrogenous heterocyclic compounds represented by the following formula: ##STR00002## in which R1-R8 each is independently a hydrogen atom; a straight or branched chain C1-12 alkyl group; a C3-12 cycloalkyl group; a C7-12 arylalkyl group; a C6-12 aryl group; a C7-12 alkylaryl group; a halogen atom; a nitro group; a cyano group; an amino group; a C1-10 alkyl group, C7-10 arylalkyl group, C3-10 cycloalkyl group, C6-10 aryl group or C7-10 alkylaryl group containing O, S, N or a carboxyl group; or a salt group containing O, S, N or a carboxyl group.

4. The process according to claim 3, wherein the co-catalyst is a carbazole compound selected from the group consisting of carbazole, 3,6-diaminocarbazole, 3,6-dibromocarbazole, 2-acetylcarbazole and 2-hydroxybenzo[a]carbazole-3-carboxylic acid sodium salt.

5. The process according to claim 1, wherein the molar ratio of the co-catalyst to the catalyst is 10:1 to 1:10.

6. The process according to claim 5, wherein the molar ratio of the co-catalyst to the catalyst is 5:1 to 1:5.

7. The process according to claim 1, wherein the metal concentration of the catalyst is 100-8000 ppm.

8. The process according to claim 7, wherein the metal concentration of the catalyst is 200-2000 ppm.

9. The process according to claim 1, wherein the reaction is carried out at a temperature of 60-140.degree. C.

10. The process according to claim 9, wherein the reaction is carried out at a temperature of 70-

100.degree. C.

11. The process according to claim 1, wherein the reaction is carried out at a pressure of 5-80 kg/cm.sup.2.

12. The process according to claim 11, wherein the reaction is carried out at a pressure of 6-12 kg/cm.sup.2.

13. The process according to claim 2, wherein the co-catalyst is one or more nitrogenous heterocyclic compounds represented by the following formula: ##STR00003## in which R1-R8 each is independently a hydrogen atom; a straight or branched chain C1-12 alkyl group; a C3-12 cycloalkyl group; a C7-12 arylalkyl group; a C6-12 aryl group; a C7-12 alkylaryl group; a halogen atom; a nitro group; a cyano group; an amino group; a C1-10 alkyl group, C7-10 arylalkyl group, C3-10 cycloalkyl group, C6-10 aryl group or C7-10 alkylaryl group containing O, S, N or a carboxyl group; or a salt group containing O, S, N or a carboxyl group.

14. The process according to claim 13, wherein the co-catalyst is a carbazole compound selected from the group consisting of carbazole, 3,6-diaminocarbazole, 3,6-dibromocarbazole, 2-acetylcarbazole and 2-hydroxybenzo[a]carbazole-3-carboxylic acid sodium salt.

Description

FIELD OF THE INVENTION

The present invention relates to a process for producing diaryl carbonates, which is to synthesize diaryl carbonates by oxidative carbonylation of phenols with carbon monoxide and oxygen, and in particular, to synthesize diphenyl carbonate from phenol.

BACKGROUND TO THE INVENTION

Diphenyl carbonate (DPC) is a less-toxic and contamination-free organic substance and an intermediate of important engineering plastic materials, and can be used in the synthesis of many important organic compounds and macromolecule materials, such as monoisocyanates, diisocyanates, polycarbonates, methyl parahydroxybenzoates, poly(aryl carbonates), etc., and as a plasticizer and solvent for polyamides and polyesters.

Recently, with the development in non-phosgene synthesis of high quality polycarbonate (PC) by using diphenyl carbonate and bisphenol A as the raw materials, diphenyl carbonate becomes a most attention-getting compound. The production of polycarbonate mostly adopts the method of polymerizing bisphenol A with phosgene or methyl chloroformate in a two-phase system of methylene chloride-water (also known as Interfacial Polymerization); however, phosgene and methyl chloroformate are very toxic substances, which will contaminate the environment severely and corrode the equipment. On the contrary, the synthesis of polycarbonate from diphenyl carbonate can avoid using toxic solvents and chlorine-containing materials so as to reduce the corrosion of equipment and contamination of environment.

Currently, there are three main methods to synthesize diphenyl carbonate: the phosgene method, the

ester exchange method and the method of oxidative carbonylation of phenol. The phosgene method is the earliest method and also the main method for producing diphenyl carbonate in the past. However, this method is complex in its process, high in cost and poor in quality, and the phosgene is very toxic and contaminates the environment severely. Thus, in foreign countries, the phosgene method has been weeded out. The ester exchange method uses dimethyl carbonate (U.S. Pat. No. 4,410,464) or dimethyl oxalate (JP 08-325207) so as to avoid the use of phosgene; however, its equilibrium conversion is low, the recovery of homogenous catalysts is difficult and it requires special reaction equipment. The method of oxidative carbonylation of phenol uses carbon monoxide, oxygen, phenol directly to synthesize diphenyl carbonate in one step. This method has a simple process, uses cheap raw materials and does not contaminate the environment, which is an attractive process route and is well worth further developing and researching.

U.S. Pat. No. 4,096,168 of General Electric Company discloses a diaryl carbonate process, comprising phenol, carbon monoxide, a base, and a Group VIIIB metal compound having an oxidation state greater than zero used as the catalyst, wherein said base is a sterically hindered amine. U.S. Pat. No. 4,096,169 also discloses that this reaction system can be carried out in the absence of any solvent, when phenols play a dual role of reactant and solvent, or in the presence of a solvent, and a suitable solvent can be methylene chloride, toluene, diphenylether, chlorobenzene, o-dichlorobenzene, etc. In addition, the base in the catalytic system can be an organic or inorganic base, such as alkali metals or alkaline earth metals and their hydroxides, quaternary ammonium and phosphonium, primary, secondary or tertiary amines, etc. Because this catalytic system cannot be re-oxidized to its original oxidation number after the oxidation state of the Group VIIIB metal having an oxidation state greater than zero reduces to zero as the reaction carries out, the reaction terminates. Also, this process uses organic solvents, which may cause contamination.

U.S. Pat. No. 4,349,485 discloses a diaryl carbonate process, comprising phenol, carbon monoxide, a base and a Group VIIIB metal, and further comprising an oxidant and a redox co-catalyst of manganese tetradentates. The manganese tetradentates are of the formula (L).sub.xMn wherein L is bis(.beta.-diketone) (C.sub.14-20H.sub.22-34O.sub.4), the oxidant is air, and a molecular sieve and tetrabutylammonium bromide are used as the drying agent and the phase transfer agent, respectively. The reaction time of this process is 80 hr and the convertibility of phenol is about 50%, which reactivity is too low.

U.S. Pat. No. 5,132,447 discloses the use of a homogenous catalytic system of palladium (II) acetate/cobalt (II) diacetate/tetra-n-butylammonium bromide, with benzoquinone added, to increase the yield of diphenyl carbonate from 15.2% to 26.1% at a high pressure (the maximum pressure is up to 2050 psi). U.S. Pat. No. 5,284,964 discloses the finding that the yield of diphenyl carbonate can achieve 45% by using palladium (II) acetate as the main catalyst, cobalt di-(salicylal)-3,3'-diamino-N-methyldipropylamine (CoSMDPT) as the inorganic co-catalyst, tetraalkylammonium bromide or hexaalkylguanidinium bromide as the source of bromides in the presence of the organic co-catalyst of terpyridine and introducing carbon monoxide and oxygen in a fixed ratio at a high pressure (the maximum pressure is up to 1600 psi). In order to achieve commercially acceptable reaction rate and selectivity, this process must be carried out at a high pressure. However, under the condition that the total reaction pressure increases continuously, the equipment investment cost will be increased greatly when commercialization.

EP 350,700 uses a cobalt salt as the inorganic co-catalyst with a quinine or hydroquinone added as the electron transfer catalyst. However, in this process, the removal of electron transfer catalyst is

extremely costly. The two OH groups provided by hydroquinone will also cause the phenol to form byproducts of carbonates, and the removal of such byproducts is costly. Also, the electron transfer catalyst cannot be recovered for reuse and the formation of byproducts lowers the selectivity. Thus the economic burden increases.

The process disclosed by JP 04-257546 is carried out in a distillation tower, which uses noble metals and quaternary salts as the catalytic system and removes reaction water by distillation. Due to the equipment problem, the holdup time is very short so that the space-time yield (STY) is very low and is merely 17.8 g/1 h. Also, a large amount of halogen ions exist in the catalytic system used by this process, which will cause corrosion.

U.S. Pat. No. 5,498,742 uses palladium bromide/tetrabutylammonium bromide/manganese(II) acetylacetonate/sodium phenolate as the catalytic system. However, the catalyst should be activated with a large amount of carbon monoxide first, which is not economically beneficial.

SUMMARY OF THE INVENTION

In view of the aforementioned problems, the main object of the present invention is to provide a process for producing diaryl carbonates, which has high reaction convertibility at a low reaction pressure.

Another object of the present invention is to provide a process for producing diaryl carbonates, which has high reaction selectivity.

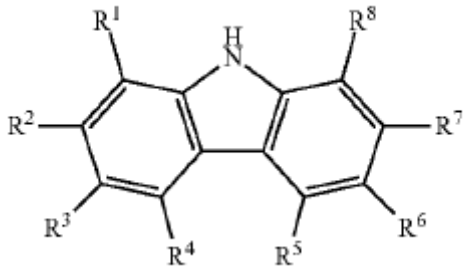
Yet another object of the present invention is to provide a process for producing diaryl carbonates, which has high reaction convertibility.

Yet another object of the present invention is to provide a process for producing diaryl carbonates, which has high reactivity.

The process for producing diaryl carbonates according to the present invention is to synthesize diaryl carbonates by oxidative carbonylation of phenols with carbon monoxide and oxygen in the presence of a catalytic system comprising Group VIIIB metal halides in combination with one or more nitrogenous heterocyclic compounds as the organic co-catalyst.

In particular, the present invention is to synthesize diphenyl carbonates by oxidative carbonylation, in which a catalytic system comprising a palladium halide catalyst in combination with one or more nitrogenous heterocyclic compounds as the organic co-catalyst is used to catalyze phenol.

The process for producing diaryl carbonates according to the present invention is characterized in that the medium for oxidative carbonylation comprises the following components: (1) a metal halide catalyst, (2) phenol, (3) a base, (4) an inorganic co-catalyst, (5) a quaternary ammonium halide, (6) carbon monoxide, (7) oxygen, and (8) an organic co-catalyst. The metal halide catalyst can be palladium halide such as, for example, palladium chloride. The organic co-catalyst can be one or more nitrogenous heterocyclic compounds represented by the following formula:



In the formula, R^1-R^8 each is independently a hydrogen atom; a straight or branched chain C_{1-12} alkyl group; a C_{3-12} cycloalkyl group; a C_{7-12} arylalkyl group; a C_{6-12} aryl group; a C_{7-12} alkylaryl group; a halogen atom; a nitro group; a cyano group; an amino group; a C_{1-10} alkyl group, C_{7-10} arylalkyl group, C_{3-10} cycloalkyl group, C_{6-10} aryl group or C_{7-10} alkylaryl group containing O, S, N or a carboxyl group; or a salt group containing O, S, N or a carboxyl group.

In particular, the organic co-catalyst is a nitrogenous heterocyclic compound of carbazoles, and the examples of the organic co-catalyst of carbazoles include, but are not limited to, carbazole, 3,6-dichlorocarbazole, 3,6-dibromocarbazole, 2-acetylcarbazole and 2-hydroxybenzo[a]carbazole-3-carboxylic acid sodium salt.

According to the present invention, the catalytic system is composed of a metal halide, especially palladium halide, and one or more nitrogenous heterocyclic compounds as the organic co-catalyst, and diphenyl carbonate is synthesized from phenol by carrying out the oxidative carbonylation in a 1 L high pressure reactor. The reaction temperature is 60-140.degree. C., and preferably 70-100.degree. C.; the reaction pressure is 5-80 kg/cm.sup.2, and preferably 6-12 kg/cm.sup.2; the molar ratio of the co-catalyst to the catalyst is 10:1 to 1:10, and preferably 5:1 to 1:5; and the metal concentration of the catalyst is 100-8000 ppm, and preferably 200-2000 ppm.

The features and effects of the present invention will be further explained with reference to the preferred embodiments below, which are, however, not intended to restrict the scope of the present invention.

DESCRIPTION OF PREFERRED EMBODIMENTS

The convertibility, selectivity and yield used in the specification are calculated according to the following equations: Convertibility (%)=Amount of Consumed Phenol (mol)/Amount of Added Phenol (mol).times.100% Selectivity (%)=2.times.Amount of Produced DPC (mol)/Amount of Consumed Phenol (mol).times.100% Yield (%)=Convertibility (%).times.Selectivity (%).times.100%

COMPARATIVE EXAMPLE

In a 1 L stainless steel high pressure reactor with stirrer, 231.72 g (2.4 mol) of phenol, 0.35 g (0.00139 mol) of manganese acetylacetonate, 3.87 g (0.012 mol) of tetrabutylammonium bromide and 0.35 g (0.00878 mol) of sodium hydroxide were added. A catalyst of palladium chloride was added so that the amount of palladium was 265 ppm based on the total amount of reactants. The air in the reactor was replaced with a mixed gas of carbon monoxide and oxygen, followed by starting the stirrer to pressurize

the reactor to 10 kg/cm.sup.2 and elevate the temperature of the reaction system to 80.degree. C. The volume ratio of oxygen/carbon monoxide was 5/95 during the reaction, and the pressure of the reactor was kept at 10 kg/cm.sup.2. Samplings were conducted at 60 minutes after the reaction was initiated. The samples were analyzed with gas chromatography. The result is shown in Table 1.

Examples 1-5

The steps of the Comparative Example were repeated except that different organic co-catalysts were added and the molar ratio of the organic co-catalyst to the catalyst was 1:1. The results are shown in Table 1. It is shown that, in a certain extent, the yields are all increased when the palladium chloride catalyst is used in combination with different co-catalysts.

TABLE 1

The benefit of palladium chloride in combination with different cocatalysts to the improvement on the yield of diphenyl carbonate

	Cocatalyst	Convertibility (%)	Selectivity (%)	Yield (%)
CEx.	none	5.9	98.9	5.8
Ex. 1	carbazole	7.2	100.0	7.2
Ex. 2	3,6-dibromocarbazole	10.3	99.1	10.2
Ex. 3	3,6-diaminocarbazole	10.4	100.0	10.4
Ex. 4	2-acetylcarbazole	8.4	99.3	8.3
Ex. 5	2-hydroxybenzo[a]carbazole-3-carboxylic acid sodium salt	9.0	99.3	8.9

CEx. = Comparative Example
Ex. = Example

Examples 6-7

The steps of the Comparative Example were repeated except that palladium chloride was used in different concentrations and the co-catalyst of 3,6-dibromocarbazole was used in a molar ratio of 1:1 with respect to the catalyst. The results are shown in Table 2. It is shown that the co-catalyst will benefit the production of diphenyl carbonate under different concentrations of the palladium chloride catalyst.

TABLE 2

The influence of the cocatalyst on the synthesis of diphenyl carbonate under different concentrations of palladium halide

	Pd concentration (ppm)	Convertibility (%)	Selectivity (%)	Yield (%)
Ex. 2	265	10.3	99.1	10.2
Ex. 6	132	7.0	99.1	6.9
Ex. 7	1000	6.8	98.9	6.7

Ex. = Example

Example 8

The steps of the Comparative Example were repeated except that the reaction was carried out at a different reaction pressure and the co-catalyst as used was 3,6-dibromocarbazole. The result is shown in Table 3. It is shown that, with the use of the co-catalyst of the present invention, a higher yield than that of the original system can still be obtained at different pressures.

TABLE 3

The influence of pressure on the production of diphenyl carbonate

	Reaction pressure (kg/cm^2)	Convertibility (%)	Selectivity (%)	Yield (%)
Ex. 2	10	10.3	99.1	10.2
Ex. 8	8	6.5	98.8	6.4

Ex. = Example

Example 9

The steps of the Comparative Example were repeated except that the reaction was carried out at a different reaction temperature and the co-catalyst as used was 3,6-dibromocarbazole. The result is shown in Table 4. It is shown that, with the use of the co-catalyst of the present invention, a higher yield than that of the original system can still be obtained at relatively-higher temperatures.

TABLE 4

The influence of temperature on the production of diphenyl carbonate

	Reaction temperature (° C.)	Convertibility (%)	Selectivity (%)	Yield (%)
Ex. 2	80	10.3	99.1	10.2
Ex. 9	90	7.5	99.0	7.4

Ex. = Example

Examples 10-11

The steps of the Comparative Example were repeated except that the reaction was carried out with different molar ratios of the co-catalyst to the catalyst and the co-catalyst as used was 3,6-dibromocarbazole. The results are shown in Table 5. It is shown that a higher yield of diphenyl carbonate than that of the original system can still be obtained under different molar ratios of the co-catalyst to the catalyst

TABLE 5

The influence of the ratio between the cocatalyst and the Pd catalyst on the production of diphenyl carbonate

	Cocatalyst/Pd catalyst	Convertibility (%)	Selectivity (%)	Yield (%)
CEx.	no cocatalyst added	5.9	98.9	5.8
Ex. 2	1/1	10.3	99.1	10.2
Ex. 10	1/2	7.2	99.1	7.1
Ex. 11	2/1	7.9	99.2	7.8

CEx. = Comparative Example
Ex. = Example

Appendix C: Thermodynamic and Equilibrium Data for Diphenyl Carbonate (DPC)

Appendix C: Thermodynamic and Equilibrium Data for Diphenyl Carbonate (DPC)

To accurately model the vapor-liquid equilibrium behavior of DPC in ASPEN Plus, the thermodynamic parameters and activity coefficients of DPC were manually inputted, as DPC is not included in the ASPEN Plus databse. The non-random two liquid (NRTL) activity coefficient model, which assumes ideal gas behavior, was used because this process is run under relatively low pressures (0.01-10 bar). To obtain the liquid-phase activity coefficient of each of the components involved in this process, the fugacity of the pure species and the NRTL parameters obtained from binary data was needed. Pure species data and binary data for all species other than DPC were obtained from the Dortmund data bank.

Using ASPEN's built-in property estimator, the pure species thermodynamic parameters of diphenyl carbonate were estimated from its molecular structure and known properties such as melting point, boiling point, and vapor pressure, which were manually inputted. The binary equilibrium data in which diphenyl carbonate is one of the components was obtained from literature sources. Using these coefficients, the ternary liquid-liquid equilibrium for diphenyl carbonate-phenol-water was reproduced reliably. Table XXIX gives the activity coefficients derived from the NRTL model.

Table XXIX: Calculated NRTL parameters for DPC

Component i								
	PHENOL	PHENOL	PHENOL	WATER	WATER	CO	DPC	DPC
	WATER	CO	O2	CO	O2	O2	PHENOL	WATER
Temperature units	F	F	F	F	F	F	F	F
Source	USER	USER	USER	USER	USER	USER	USER	USER
Property units:								
aij	0	0	0	0	0	0	-2.843	1.781
aji	0	0	0	0	0	0	0.1393	6.390
bij	-407.41	-813.914	-773.967	-201.875	-183.295	-33.84	0	0
bji	1798.91	277.882	231.047	327.31	314.168	34.27	0	0
cij	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
dij	0	0	0	0	0	0	0	0
eij	0	0	0	0	0	0	0	0
eji	0	0	0	0	0	0	0	0
fij	0	0	0	0	0	0	0	0
fji	0	0	0	0	0	0	0	0
Tlower	77	77	77	77	77	77	-459.67	-459.67
Tupper	77	77	77	77	77	77	1340.33	1340.33

Figure 12 shows the ASPEN-generated ternary diagram for the DPC-phenol-water system based on the calculated coefficients above. This diagram matches those found in the literature, indicating that these calculated coefficients are reliable.

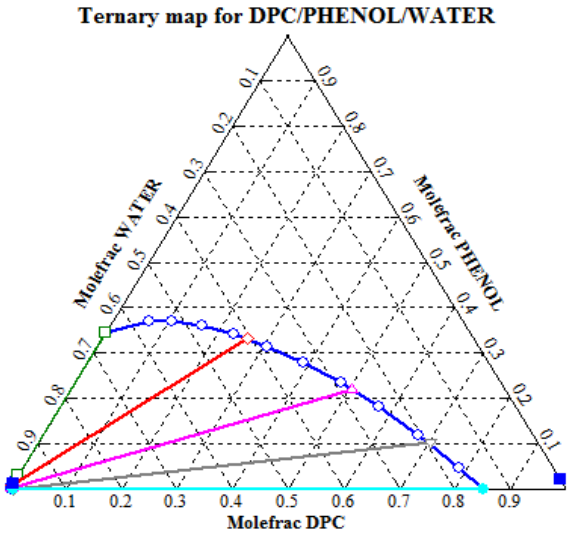


Figure 12: ASPEN Plus-generated ternary diagram for the DPC-phenol-water system

Appendix D: Sample Calculations for Equipment Sizing and Costing

Appendix D1: Sample Calculation for Distillation Tower Size and Price

Equipment: Distillation Tower D1

Design Specifications

Material	Column Type	Packing Type	HETP
Carbon Steel	Packed	Sulzer Mellapack	1.417 ft

Flow Rates

Molar Reflux Ratio	Distillate rate	Liquid Rate
0.65125	1200.0 ft^3/hr	193.09 ft^3/hr

Operating Parameters

Pressure	Temperature	R [ft^3.psi/R.lbmol]	Vapor Density
10 psig	207 C	10.73159	.01213 lb/ft^3

Flooding Velocity (U_f) *[ft/sec]*

F_{st} = (surface tension/20)^.4 = 1

F_{HA} = 1; sieve trays with A_b/A_A = .1 Plate Spacing = 11 in

F_f = 1 (non-foaming system) C_{sb} = .28

$F_{lg} = (L/V)(\rho_v/\rho_L)^{.8}$ = .01626 ρ_L = 67.328 lb/ft^3

$U_f = C_{sb}F_{st}F_fF_{HA}(\rho_L-\rho_v)^{.5}(\rho_v)^{-.5}$ = .339 ft/s U = .85 * U_f = .2883 ft/s

Column Size

Packed Diameter	Tray Diameter	Height	# of Trays
15.58 ft	17.18 ft	40 ft	14

Column Purchase Price

Corrosion Allowance	Weld Efficiency	Vessel Wall Thickness
.25 in	0.85	1.050 in

Fm: Carbon Steel	ρ_{CS}	Height of packing
1	490 lb/ft^3	19.838 ft

Weight Factor = = 110717 lbs.

$C_v = EXP\{7.2759 + 0.18255LN(W) + 0.02297LN(W)^2\}$ = $ 234,231.62

C_{pl} (platforms & ladders) = 300.9 x $(D_i^{0.63316})$ x $L^{.80161}$ = $32,940.90

Vol. of Packing: 3782.01 ft^3 Cost/ft^3 =$122.60 $C_{l(packing)}$ = $ 463,682.28

Final Cost Calculations

$C_p = F_mC_v + C_{pl} + C_l$	CE Index	Bare-Module Factor	C_b
$763,507.36	585.6	4.16	$3,719,952.70

Appendix D2: Sample Calculation for Condenser

Equipment: Condenser 1

Design Specifications

Material	Exchanger Type	Head Type	Length
Carbon Steel	Shell and Tube	Floating	20 ft

Tube Inside Diameter	Pitch Type
1 in.	Square

Sizing Considerations

Heat Duty (Q)	Hot Stream In	Hot Stream Out	$DeltaT_{lm}$
(-)426146 BTU/hr	80.0 C	25.0 C	15.91

Cold Stream In	Cold Stream out
20.0 C	60.00 C

U (BTU/hr.ft^2.F) = 70.725

Heat Exchange Surface Area, A (ft^2) = Q / DeltaTlm x U = 11.0928

Costing Condenser

Fm	Fl	C_b = EXP[11.667 - 0.8709x(ln(A)) + 0.09005x(ln(A))^2]
1	1	$25804.25

$F_p = 0.9803 + 0.018 \times (P/100) + 0.0017 \times (P/100)^2 = 1.02$

$C_p = F_m \times F_p \times F_l \times C_b$	CE Index	Bare Module Factor	C_{bm} Cost
$32,744.63	585.6	3.17	$124,002.54

Appendix D3: Sample Calculation for Pump and Electric Motor

Equipment: Pump 1 and Electric Motor 1

Design Specifications

Material	Pump Type	Flow Rate, Q	Pressure Change
Stainless Steel 316	Centrifugal	8.09 gal/min	202.91 psi

Input Stream Density	Head	F_t	F_m
69.0274 lb/ft^3	423.29 $ft.lb_f/lb$	1	2

Additional Specs

Shaft Rotation	No. of Stages
3600 rpm	1

Pump Sizing

Power Requirement, P_t (Hp) = [(vol. rate)(Pressure increase) x 144] / (3600 x 550.22) = 0.1648

Size Factor, S ($gpm.ft^{.5}$) = $Q\,(H)^{.5}$ = 166.31

C_b = EXP [9.7171 - 0.6019(ln(S)) + 0.0519$(ln(S))^2$] = $ 2970.05

CE Index	Bare Module Factor	C_{bm}
585.6	3.3	$11,479.12

Motor Sizing

Type	Shaft Rotation	F_t
Explosion Proof	3600 rpm	1.8

Brake Power, P_b	Fluid Power	Electricity
0.16483 hp	0.048733 hp	0.1229 kW

Pump Efficiency, η_p = -.0316 + .24015 (lnQ) - .01199$(lnQ)^2$ = .2957

Motor Efficiency, η_m = 0.8 + 0.0319(lnP_b) - 0.00182$(lnP_b)^2$ = .792

Power Consumption of Motor = $P_t / (\eta_p * \eta_m)$ = 9.00 Hp

CB = EXP{5.8259 + 0.13141(lnP_c) + .053255$(lnP_c)^2$ +.028628$(lnP_c)^3$ - .035549$(lnP_c)^4$} = $ 1504.5

$C_p = F_T \times C_B$	CE Index	Bare Module Factor	C_{BM}
$2,708.10	585.6	3.3	$10,435.39

Total Purchase Cost: $21914.52

Appendix D4: Sample Calculation for a Flash Drum

Equipment: Flash Column 1

Design Specifications

Material	Column Type	Residence Time, τ	Aspect Ratio, AR
Stainless Steel 316	Horizontal	4 min	4

Fraction of Drum Full	K Factor	Vapor Density	Liquid Density
0.5	0.27	0.823 lb/ft^3	64.446 lb/ft^3

Flow Rates

Volumetric Flow, Q	Vapor Fraction
27947 ft^3/hr	0.29567

Operating Parameters

Pressure	Temperature	R (ft^3.psi/R.lbmol)
145.04 psia	207 C	10.73159

Vessel Sizing

Volume (ft^3) = (Q)(τ) / 60 = 1863.13

Length: 13.1 ft

Diameter (ft) = (4*volume/AR)$^{1/3}$ = 5.241

Vessel Costing

Corrosion Allowance (in)	Min. Wall Thickness	Density of Material	FM
0.25	0.5	489 lb/ft^3	2

W (lbs) = π (D_i + t_s)(L + 0.8D_i) x t_s x ρ_{ss} = 14818.19

C_V = EXP{8.9552 - .2330ln(W) + 0.04333ln(W)^2} = $167,881.42

Additional Costs

C_{PL} (Platforms & Ladders) = 2005(D_i)$^{0.20294}$

$2,806.16

$C_P = F_M$ x C_V + C_{PL}	CE Index	Bare Module Factor	C_{BM}
$170,687.58	585.6	3.05	$743,308.57

Appendix D5: Sample Calculation for a Storage Tank

Equipment: Storage Tank 1

Design Specifications

Material	Aspect Ratio, AR	Storage Needed
Incoloy-825	3	216,203.7 gal

Material Density (ρ)	Pressure	Welding Efficiency
0.294 lb/in^3	217.55 psi	0.85

Material Tensile Strength	Temperature	Material Factor (F_m)
101,526 psi	100C	3.7

Vessel Sizing

$V_{tank} = V_{needed}/.75$	$D_i = ((4/3\Pi)*V_{tank})^{1/3}$	$L = 3D_i$
288272 gal	25.38 ft	76.14 ft

$P_{design} = EXP\{.60608 + .91615\ln(P) + .0015655[\ln(P)]^2\} = 265.74$ psig

Minimum Thickness Req (t_p) $= (P_d*D_i/2SE - 1.2P_d) = .4$ in

Thickness Suggested (t_s)	Weight (W) $= \pi(D + t)(L + 0.8D)(t_s)(\rho)$
0.625 inches	196,654 lb

Costing

Empty Vessel Cost (C_v)$= F_m(EXP\{ 8.9552 - .2330\ln(W) + .02297\ln(W)^2\}$

$1,046,825

Ladder Cost (C_{pL}) $= 2005(D_i)^{.20294}$	Purchase Cost (C_p) $= (F_m)(C_p) + (C_{pL})$
$3,865	$1,050,690

Total Bare-Module Cost $= 3.05C_p$

$3,753,232

Appendix D6: Sample Calculation for a Heat Exchanger

Equipment: Heat Exchanger 1 (F2-HX1)

Design Specifications

Material	Exchanger Type	Head Type	Length
Carbon Steel	Shell and Tube	Floating	20 ft

Tube Inside Diameter	Pitch Type	Shell Inside Diameter
1 in.	Square	15.25 in.

Aspen Values

Cold Stream Flow, V_c	Hot Stream Flow, V_h	Heat Duty, Q	U_i
56154.72 kg/hr	50266.4 kg/hr	(-)19,989,895.4 BTU/hr	95 BTU/ft2.hr.C

Sizing Considerations

Hot Stream In	Hot Stream Out	DeltaTlm =
88.2 C	83.096 C	{$DeltaT_a$ - $DeltaT_b$/ln($DeltaT_a$/$DeltaT_b$)} 63.14798573

Cold Stream In	Cold Stream out
20.0 C	25.0 C

$S = (T_{c,o} - T_{c,i}) / (T_{h,i} - T_{c,i})$	$R = (T_{h,i} - T_{h,o}) / (T_{c,o} - T_{c,i})$	Fouling Factor, F_t
0.073313783	1.0208	0.91

Total tube inside area, A (ft^2) = Q / ($deltaT_{lm}$ x U x F_t) = 3661.73

Estimated Velocity, v_i: 5 ft/s inside tube

Total cross sect. area per pass, A_{ct} (ft^2) = V_c / ($\rho_{cold\ stream}$)(v_i)(3600) = .0781

Heat Exchange Surface Area, A (ft^2) = 3941.81

No. of tube passes, $N_p = A_t/(A_tN_t)$ = 1.12 or 1

No. tubes/pass, $N_t = 4A_{ct}/ \pi D_t^2$ = 11.7 or 12

Estimated Baffle Spacing, b	Shell Side Pressure, P
10 in.	15 psia

Costing Heat Exchanger

F_m	F_l	C_b = EXP[11.667 - 0.8709x(ln(A)) + 0.09005x(ln(A))^2]
1	1	$52,971.34

$F_p = 0.9803 + 0.018 \times (P/100) + 0.0017 \times (P/100)^2 = .99$

$C_p = F_m \times F_p \times F_l \times C_b$	CE Index	Bare Module Factor	C_{bm}
$52,441.63	585.6	3.17	$194,700.25

Appendix D7: Sample Calculation for a Reactor

Equipment: Reactor 1 (R1)

Design Specifications	Material	Vessel Type	Residence Time	Aspect Ratio, AR
	Stainless Steel 316	Horizontal	63.15 min	2
Operating Parameters	Pressure	Temperature	R (ft^3.psi/R.lbmol)	
	145.04 psia	80 C	10.73159	
Reactor Sizing	Input Streams	Volume of Vessel, V		
	56914.06 ft3/hr	29951.02	ft^3	
	$V = \pi D_i^2 * (1/4) * L$	and $L = (AR)\ D_i$ so…	$Di = [4 \times V / (2 \times \pi)]^{1/3}$	Length
			26.72 ft	53.43 ft
Vessel Costing	Corrosion Allowance (in)	Min. Wall Thickness	Density of Material	F_M
	0.25	0.5	489 lb/ft^3	2
	$W\ (lbs) = \pi[Di + t_s)(L + 0.8D_i) \times t_s \times \rho_{ss} = 256{,}643.60$			
	$C_v = EXP\{8.9552 - .2330\ln(W) + 0.04333\ln(W)^2\} = \$353{,}350.04$			
	C_{PL} (Platforms & Ladders) = 2005(Di)0.20294			
	$3,905.37			
	$C_P = F_M \times C_V + C_{PL}$	CE Index	Bare Module Factor	C_{BM}
	$745,940.45	585.6	3.05	$2,664,618.63
Agitator Costing	Categorization: For gas dispersion into a liquid			
	Requirement	Volume of Vessel	HP Needed, P	
	10 HP /1000 gal	224049 gal	2240.49	
	C_p Agitator*	CE Index	Bare Module Factor	C_{BM}
	$100,000.00	666.5	1.5	$199,950
Agitator Motor	Steam Turbine	$C_p = 9400 \times (P^{.41})$		
	Non-Condensing	$222,212.50		

	CE Index	Bare Module Factor		C_{BM}
	585.6	1		$260,255.28
Heating Coils	Heuristic*	C_p		C_{BM}
	10% of Reactor C_p	$87,364.55		$87,364.55
			Total Cost:	$3,212,188.45

Appendix D8: Sample Calculation for a Vacuum Pump

Equipment: Vacuum Liquid Ring Pump 1 (VAC1)

Design Specifications

Material	Pump Type	Flow Rate, Q	Pressure Change
Stainless Steel	Liquid Ring	234890 ft^3/hr	22.5 Torr

Air leakage flow

A = 20 lb/hr (read off chart)

Power Requirement

Pt (Hp) = [(vol. rate)(Pressure increase) x 144] / (3600 x 550.22) = 683.88

Pump Sizing

S = (HP + A) / Pressure Change = 25.75 ft3/min

C_b = EXP [9.7171 - 0.6019(ln(S)) + 0.0519(ln(S))2] = $47,680.18

Utility Costs

Notes: *Same electricty costs referenced previously in report*

Operation for 8620 hr/yr

Oil sealed mechanism

Utility Cost: $219,797.07

Bare Module Factor	Total Cost / yr
1	$267,477.25

Appendix E: Distillation Tower Design

Appendix E: Distillation Tower Design

Once the DPC production process had been designed, the optimal operating conditions for each block needed to be specified. Both distillation towers were optimized and sized in ASPEN Plus, which used the "Design Specification" feature to return the optimal reflux ratio for a range of number of stages and feed tray locations.

The first distillation tower, D1, separates DPC, the bottoms product, from water and phenol, the tops product. The desired specification was a 99% pure stream of DPC by mass, with phenol as the remaining 1% mass. The remainder of the phenol, along with water and trace gases, comprise the tops product. Since the inlet stream composition was known from the results of upstream blocks, a mass balance calculation was performed on the tower, as shown in Table XXX.

Table XXX: *Goal mass balance for distillation tower D1*

	TODIST1	DPC	PHOH-H2O
Temperature C	120		
Pressure bar	0.1		
Vapor Frac	0.019		
Mole Flow kmol/hr	600.003		
Mass Flow kg/hr	56940.002	5889.818182	51050.18382
Volume Flow cum/hr	2878.49		
Enthalpy MMBtu/hr	-98.569		
Mass Flow kg/hr			
PHENOL	50312.4	58.89818182	50253.50182
WATER	491.99	0	491.99
DPC	5830.92	5830.92	0
CO	304.692	0	304.692
O2	0	0	0
PALLA-01	0	0	0
Mass Frac			
PHENOL	0.884	0.01	0.98439414
WATER	0.009	0	0.00963738
DPC	0.102	0.99	0
CO	0.005	0	0.00596848
O2	0	0	0
PALLA-01	0	0	0

An ASPEN Plus file consisting only of D1 and its inlet and outlet streams was created, and the inlet stream was specified as above. The specified conditions on the tower were the bottoms rate, known as 5889.818182 kg/hr from above, and the reflux ratio, which was arbitrarily set to 1. The pressure of the top stage was specified to be 25 mmHg, the condenser pressure drop was 25 mmHg, and each stage sustained a 7.5 mmHg pressure drop. To obtain a 99% pure stream of DPC, a design specification was set up. The mass purity of the bottom stream was specified to be 99% pure DPC, and the reflux ratio was varied from 0.1 to 10. The tower sizing feature was also activated for both trayed and packed towers, with a goal of obtaining a tower diameter of less than 20 feet. For tray towers, Koch

Ballast trays were used with 2 feet between each tray. For packed towers, Mellapak standard packing with a specification of 125X was used with a HETP of 17 inches.

The simulation was run as the number of trays varied from 12 to 15 and the feed stage varied from 3 to 9. These combinations of number of trays and feed tray location were chosen because the simulation converged without errors or warnings and because the tower diameters were less than 20 feet. For each run, the following values were recorded: the optimal reflux ratio as determined by the design specification, the condenser duty, the reboiler duty, the tray tower diameter, and the packed tower diameter.

Once all of the data were collected, they were analyzed to determine the optimal tower design. For a given number of stages, the feed tray location that returned the smallest reflux ratio was determined to be the best. Of these, the tower with the lowest energy requirement and smallest diameter was selected. D1 was designed to have 14 stages, a feed tray location of tray 5, and a diameter of 11.67 ft.

The second distillation tower, which removes water in order to recycle as much pure phenol as possible, was designed in a similar process. A mass balance calculation was done based on the known inlet stream and the desired outlet streams; namely, all water and gases in the tops product and all phenol in the bottoms product, as shown in Table XXXI.

Table XXXI: *Goal mass balance for distillation tower D2*

	TODIST2	H2O	PHOH
Temperature C	25.1	99.6	193.1
Pressure bar	1.4	1	1.37
Vapor Frac	0	1	0
Mole Flow kmol/hr	551.169	25.741	525.428
Mass Flow kg/hr	49908.876	465.432	49443.444
Volume Flow cum/hr	45.924	797.793	53.728
Enthalpy MMBtu/hr	-83.688	-5.829	-59.837
Mass Flow kg/hr			
PHENOL	49443.444	1.461	49441.984
WATER	463.966	462.505	1.461
DPC	0	0	0
CO	1.466	1.466	0
O2	0	0	0
PALLA-01	0	0	0
ACETONE	0	0	0
Mass Frac			
PHENOL	0.991	0.003	1
WATER	0.009	0.994	0
DPC	0	0	0
CO	0	0.003	0
O2	0	0	0
PALLA-01	0	0	0
ACETONE	0	0	0

The design specification in this case was set to the specified tops flowrate of 465.432 kg/hr, and the reflux ratio was again varied from 0.1 to 10. The pressure of the top stage was specified to be 1 bar mmHg, the condenser pressure drop was 200 mmHg, and each stage sustained a 8.5 mmHg pressure drop. The tower sizing functions for trayed and packed towers were activated, and the conditions were the same as those for D1, except that the HETP for the packed tray sizing was 14 inches. The simulation was run for towers of 10-14 stages, where the feed tray location varied from stage 4 to stage 11. As with D1, these ranges were chosen because they converged for tower diameters of less than 20 feet. D2 was designed to have 11 stages, a feed tray location of stage 8, and a diameter of 6.80 ft.

Appendix F: Alternative Process Designs

Appendix F: Alternative Process Designs

Iteration 1

The first iteration of the DPC-producing process adapted the processes used in traditional paths to DPC to this novel reaction and is shown in Figure 13.

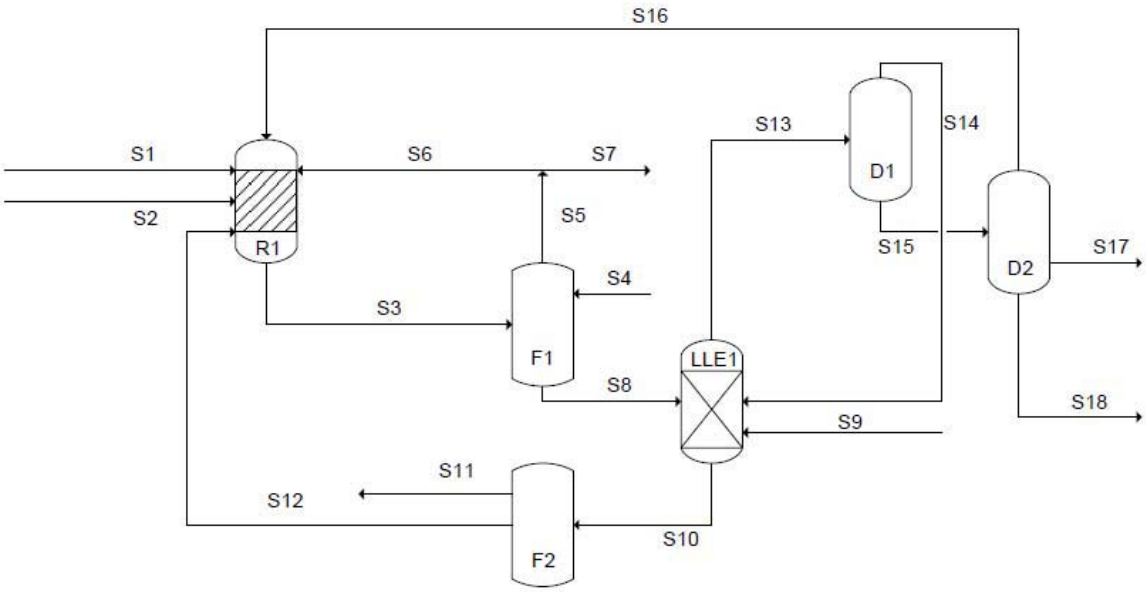


Figure 13: *First iteration of the DPC production process design*

Phenol and the catalysts are mixed together and fed continuously through stream S1. Carbon monoxide and oxygen are mixed together and fed continuously through stream S2. The reactor conditions are then adjusted to those required for the oxidative carbonylation of phenol. The mean residence time inside the reactor is 60 minutes. After the reaction in the CSTR, the effluent stream S3 is passed to a flash vessel, which introduces a stream S4 of aqueous HCl to neutralize the basic solution. The vapor product is removed through S5, and a small portion is purged through S7. Stream S6

represents a gas recycle stream for unreacted carbon monoxide. The liquid product from the flash vessel F1 is removed through stream S8. The palladium catalyst originally fed to the reactor is $PdCl_2$, which is insoluble in neutral water. Using hydrochloric acid allows $PdCl_2$ to dissolve as $[PdCl_4]^{2-}$ and separate it from the organic mixture. The liquids, including phenol, molten DPC, and the catalysts, are passed to liquid-liquid extractor LLE1, which uses an initial injection of toluene through stream S9 to separate phenol and DPC from the catalysts. Phenol and DPC would preferentially dissolve in toluene and the catalysts would preferentially dissolve in water. Since toluene and water are immiscible with each other, a decanter would be used to separate the layers. The raffinate product stream S10 contains the aqueous layer, which then passes through vaporizer F2 to remove excess water. The catalysts are then recycled back to the reactor through stream S12. The extract product stream S13 contains the organic layer which then undergoes two successive distillations in towers D1 and D2, resulting in the recovery and recycle of toluene and phenol, respectively. DPC is recovered as the bottoms product of the second distillation column D2.

Although liquid-liquid extraction followed by distillation has been proven successful in the Wacker process for the synthesis of acetaldehyde from ethylene, this design presented severe limitations that prevented it from being the most viable. First, there is not enough thermodynamic and solubility data available to determine the efficacy of the suggested solvents on how DPC and the catalysts would split between the organic and aqueous phases at the process conditions required. Second, the introduction of HCl presents a safety hazard due to corrosion and would require special containers. The use of HCl also results in the formation of NaCl, which must removed and disposed of properly as an inorganic byproduct. Finally, the introduction of various solvents introduced the possibility of producing more undesired species than the side products already unknown.

Iteration 2

The second process design, shown in Figure 14, improved upon the first by adding a second liquid-liquid extractor before the distillation towers and by replacing the vaporizer with a desalination unit. As before, the reactor effluent S3 enters a disengagement vessel F1 to recycle unreacted carbon monoxide while passing the liquid stream S7, including phenol, diphenyl carbonate, and the catalysts, to a series of two liquid-liquid extractors (LLE1 and LLE2) followed by two distillation towers (D1 and D2).

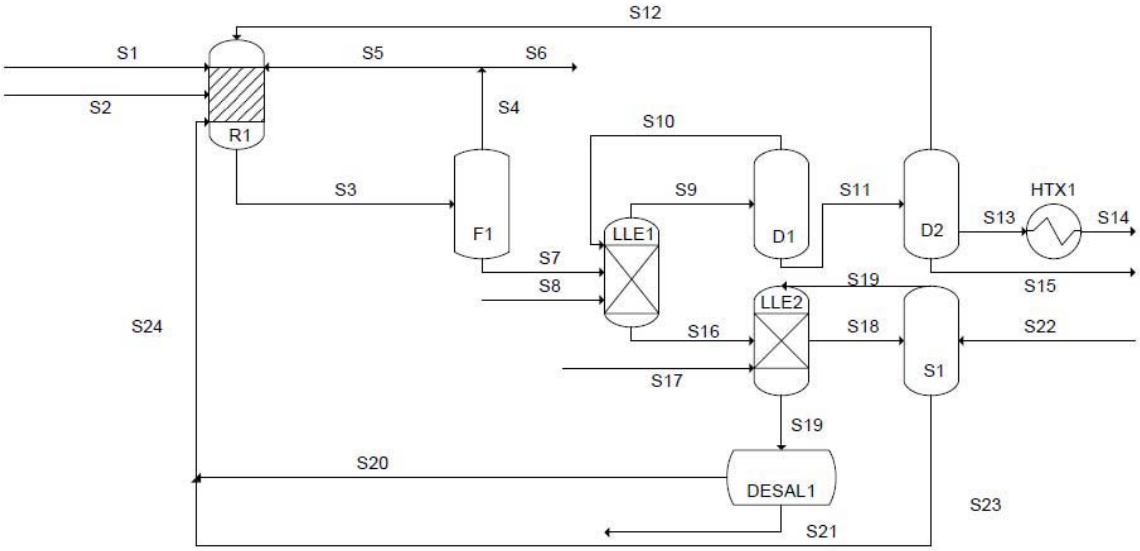


Figure 14: *Second iteration of the DPC production process design*

The solvent for the first extractor is diethyl ether with a small amount of aqueous HCl to quench the basic solution. Since both phenol and diphenyl carbonate are soluble in diethyl ether, NaCl, $PdCl_2$, and $[nBu_4]NI$ move into the aqueous phase in the first reactor, while phenol, DPC, the manganese catalyst, and the heavy side products move into the organic phase. The organic stream S9 then enters the distillation tower D1, which removes the ether and recycles it back to the extractor LLE1 through stream S10. The bottoms from D1 is fed into the second distillation tower, D2, which recycles the overhead product phenol back to the reactor through stream S12. Diphenyl carbonate is drawn from the

tray just above the reboiler stage. This process includes the additional step of removing heat from the molten DPC stream to solidify it before presenting it to the consumer.

The aqueous stream S16 from LLE1 then enters the second liquid-liquid extractor, LLE2, which separates $PdCl_2$ from NaCl and $[nBu_4]NI$. Since sulfides bind strongly with late transition metals, by employing an alkyl sulfide, palladium dichloride can be extracted from an acidic aqueous solution. The raffinate aqueous stream S19 is passed through a desalination block which removes a vast majority of salt. The aqueous desalinated stream S20 is recycled back to the reactor. The organic extract stream S18 from LLE2 then enters a stripping tower, S1, where an aqueous saturated solution of ammonia is used to recover $PdCl_2$. The alkyl sulfide is recycled to LLE2 through the stream S19 and palladium is recycled back to the reactor through stream S23.

As with the first design, there is a significant amount of uncertainty in the thermodynamic behavior of the DPC, catalysts, and solvents and how they split between aqueous and organic phases. This design also incorporates HCl, which again brings up safety concerns. However, this design introduces additional considerations that make it a non-ideal candidate. The manganese catalyst is discarded instead of recycled, which incurs the additional cost of replenishing it, and the organic ligand is split into multiple streams, where its behavior is uncertain. Furthermore, salt water is discarded, which presents an environmental hazard.

Iterations 3 and 4

The third and fourth designs incorporate only minor changes to the second design. The third design incorporates an acid quench in the flash vessel F1 immediately following the reactor R1. This was envisioned to occur by spraying the reactor effluent with an aqueous solution of HCl. The acid quench serves to neutralize the basic reactor effluent and to reduce its temperature so that the gases and liquids could separate more easily.

The fourth design adds a desiccant, in the form of a hygroscopic solid, which removes water from the reactor effluent. The solid desiccant is separated from the liquid stream by filtration, and a portion of the anhydrous organic stream is then recycled back to the reactor. The water removal step serves to drive the reaction forward and increase conversion. The option of having two reactors run in parallel was also considered so that while the desiccant in one of the reactors was being replenished, the other reactor would be operating and vice versa. Another model of this water removal process involves recycling of the desiccant. After the dehydration process, the spent desiccant would be flushed with fresh organic solvent to remove entrained catalysts and products and then treated with superheated steam to remove water from the desiccant. The dry, regenerated solid desiccant is then recycled back to the reactor. Overall, however, the same limitations that apply to the second design also apply to the third and fourth designs.

Iteration 5

The fifth design, shown in Figure 15 on the next page, expands upon the liquid-liquid extraction setup developed in the previous designs and incorporates a flash vessel, a vacuum distillation tower, and a series of liquid-liquid extractors to isolate DPC and recycle as much catalyst and unreacted reagents as possible.

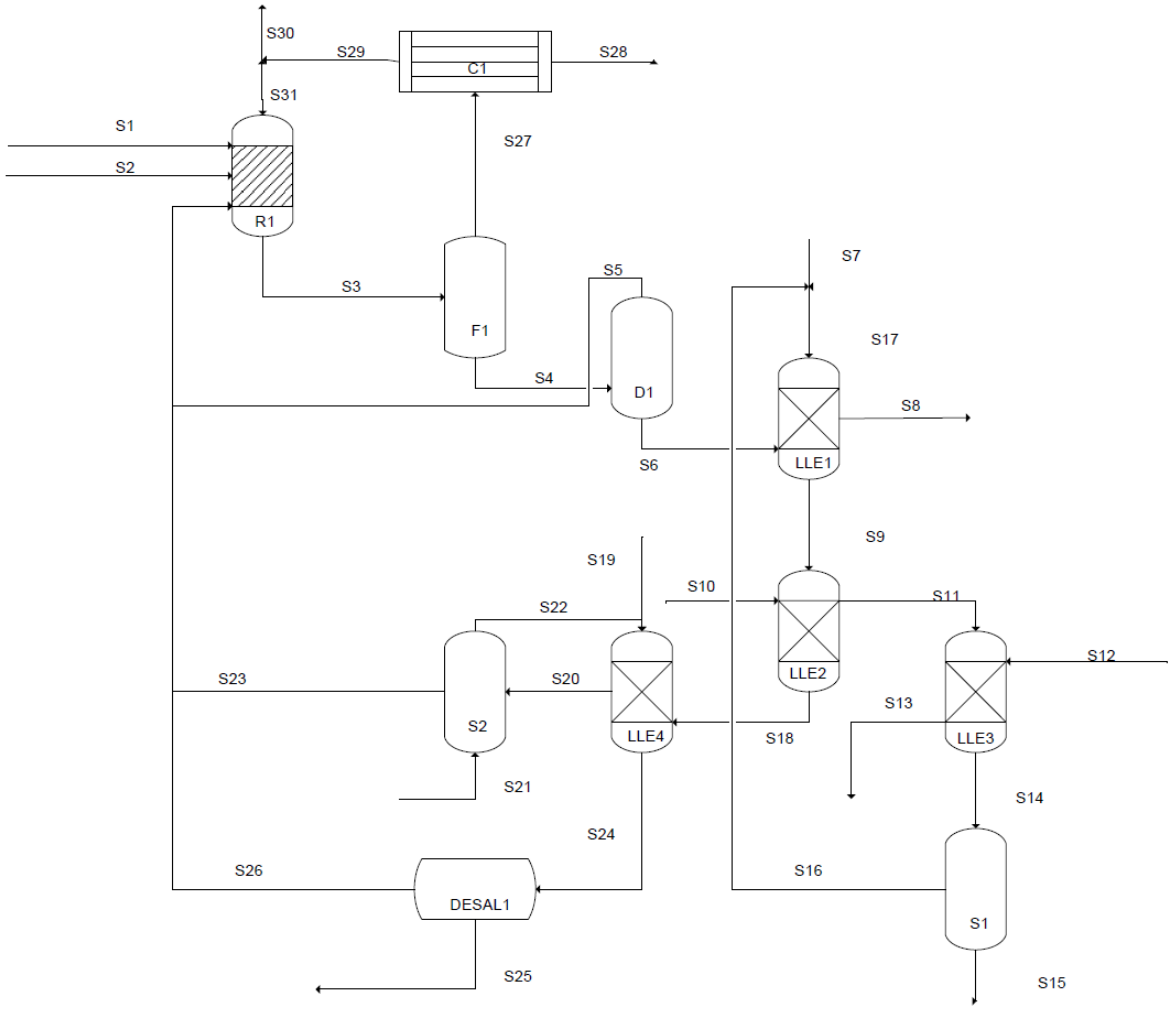


Figure 15: *Fifth iteration of the DPC production process design*

Water removal from the reactor is accomplished by simply flashing the reactor effluent so that most of the unreacted carbon monoxide and water would vaporize and separate from the liquid stream. The vapor stream leaving the flash vessel F1 enters a condenser unit that recycles carbon monoxide back while discarding water and a trace amount of phenol as the condensate. The liquid stream S4 from the flash vessel F1, which contains phenol, DPC and the catalysts, enters a vacuum distillation tower, D1,

which recycles the unreacted phenol and the remaining water to the reactor. The bottoms product contains DPC and the catalysts, and it is pumped to the first liquid-liquid extractor LLE1.

LLE1 uses diethyl ether as the extractant to separate DPC and catalysts from the inorganic byproducts. The aqueous stream is discarded, while the organic stream enters the second liquid-liquid extractor, LLE2, which uses HCl to separate the DPC and ether from the catalysts. The organic stream containing DPC enters a third liquid-liquid extractor, LLE3, which performs an aqueous wash to remove trace amounts of inorganic byproducts such as hydrochloric acid, and the DPC is isolated subsequently in solvent stripper S1. The catalyst solution S18 passes through a fourth liquid-liquid extractor, LLE4, which uses the alkyl sulfide presented in the fourth iteration of this design to separate the catalysts. The same catalyst stripper and desalination blocks are used to isolate the catalysts before recycling them back to the reactor.

Many of the same uncertainties faced in the earlier iterations of this process apply to this design as well. There is not enough thermodynamic and physical property data to determine appropriate solvents and extractants for DPC and for these catalysts. Similarly, it is unknown how the solubilities of DPC and of these catalysts in the organic and aqueous phases can be manipulated with these solvents. As a result, it is likely that DPC, water, and phenol appear in many different streams. Because the thermodynamic behavior of these compounds is unknown, the efficiency of the separator units and the purity of the streams is unknown. This leads to a lower recovery of DPC, since it would appear in many different streams, and a lower final recovery means that more fresh feed would be necessary and costs would be higher.

Appendix G: Chemical Engineering Cost Indices

Appendix G: Chemical Engineering Cost Indices

Table XXXII: *Average CE indices, as of 2012*

	Final 2012 Agrregate	Ratio
Average CE Index	585.6	1.1712
Equipment	713.9	1.4278
Hex & Tanks	661.4	1.3228
Process Machinery	666.5	1.333
Pipe, Valves, and fittings	917.7	1.8354
Process Instruments	425.1	0.8502
Pumps and Compressors	927	1.854

Appendix H: Utility Cost Summary

Table XXXIII: *Cost of steam and cooling water utilities*

	Temperature (oC)	Pressure (psi)	Flowrate (kg/hr)	Total (kg/hr)	Price in 1995($/ton)	Price in 2012 ($/ton)	Cost($/hr)	Hours/year	Cost ($/year)
Steam 1: D1 Reboiler	214.08	300	6083.41751	16770	5.94	8.90	149.31	8620	1287025.73
Steam 2: D2 Reboiler	214.08	300	10686.5524						
Steam 3	138.32	50	552.20114	552.20	6.6	9.9	5.47	8620	47123.74
C1-COOL	25	50	2330.63636	212197.8	0.02	0.03	6.37	8620	54874.35
C2-COOL	25	50	79806.9113						
R1-COOL	25	50	50853.1959						
D1-COOL	25	50	79207.0632						
							Total Cost of Utilities:		**$1,389,023.82**

Table XXXIV: Cost of electric utilities

Total energy Consumption (kWh)	Price in 1995($/kWH)	Price in 2013(kWH)	Cost($/hour)	hours/year	$/year
1351.481577	0.06	0.09	121.63	8620	**$ 1,048,479.41**

Appendix I: ASPEN Plus Simulation Report

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
PAGE 1

                              RUN CONTROL SECTION

 RUN CONTROL INFORMATION
 -----------------------

 THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

 TYPE OF RUN: NEW

 INPUT FILE NAME: _4854wft.inm

 OUTPUT PROBLEM DATA FILE NAME: _4854wft
 LOCATED IN:


 PDF SIZE USED FOR INPUT TRANSLATION:
   NUMBER OF FILE RECORDS (PSIZE) =     0
   NUMBER OF IN-CORE RECORDS      =   256
 PSIZE NEEDED FOR SIMULATION    =   256

 CALLING PROGRAM NAME:          apmain
 LOCATED IN:
C:\PROGRA~2\ASPENT~1\ASPENP~2.3\Engine\xeq

 SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

 DESCRIPTION
 -----------

        General Simulation with English Units : F, psi, lb/hr,
lbmol/hr,
        Btu/hr, cuft/hr. Property Method: None Flow basis for input:
Mole
        Stream report composition: Mole flow
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
FEED	----	R1	S1	R1	F1
S2	F1	C1	S5	F1	V1
S3	C1	S1	S10	F2	COM1
S7	F2	S2	S6	V1	F2
CATPURGE	S2	----	S8	S2	P1
COPURGE	S1	----	S4	S1	R1
H2O	D2	----	S16	D2	P3
S12	D1	C2	S19	D1	P4
S13	C2	F3	S17	P3	C4
S9	P1	R1	F3TOPS	F3	----
S14	F3	P2	S15	P2	D2
S11	COM1	D1	S20	P4	C3
FINALDPC	C3	----	S18	C4	R1

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
R1	FEED S4 S9 S18	S1
F1	S1	S2 S5
C1	S2	S3
F2	S6	S10 S7
V1	S5	S6
S2	S7	CATPURGE S8
S1	S3	COPURGE S4
D2	S15	H2O S16
D1	S11	S12 S19
C2	S12	S13
P3	S16	S17
P1	S8	S9
F3	S13	F3TOPS S14
P2	S14	S15
COM1	S10	S11
P4	S19	S20
C3	S20	FINALDPC
C4	S17	S18

CONVERGENCE STATUS SUMMARY

TEAR STREAM SUMMARY

```
   STREAM    MAXIMUM                   MAXIMUM     VARIABLE
CONV
   ID        ERROR        TOLERANCE    ERR/TOL     ID             STAT
BLOCK
   ------    -------      ---------    --------    --------       ----
-----
   S1        0.66374E-05  0.71505E-05  0.92824     CO MOLEFLOW      #
$OLVER01

   #  = CONVERGED
   *  = NOT CONVERGED
```

```
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                                FLOWSHEET SECTION

 CONVERGENCE BLOCK:  $OLVER01
 ---------------------------
     Tear Stream  :  S1
     Tolerance used:  0.100D-03
     Trace molefrac:  0.100D-05

     MAXIT=   30 WAIT   1 ITERATIONS BEFORE ACCELERATING
     QMAX =   0.0     QMIN =  -5.0
     METHOD: WEGSTEIN      STATUS: CONVERGED WITH WARNINGS
     TOTAL NUMBER OF ITERATIONS:    14


*****************************************************************************
*
     *
*
     *     STREAMS CROSSING THE CONVERGENCE LOOP NOT IN MASS BALANCE
*
     *
*

*****************************************************************************
*


                           *** FINAL VALUES ***

VAR#  TEAR STREAM VAR  STREAM   SUBSTREA COMPONEN ATTRIBUT ELEMENT
UNIT         VALUE       PREV VALUE       ERR/TOL
----  ---------------  -------- -------- -------- -------- -------- --
---------  ------------   ------------   ------------
   1  TOTAL MOLEFLOW   S1       MIXED
LBMOL/HR     1869.3650      1869.3064         0.3136
   2  MOLE-FLOW        S1       MIXED    PHENOL
LBMOL/HR     1179.4462      1179.4417      3.7497-02
   3  MOLE-FLOW        S1       MIXED    WATER
LBMOL/HR       61.8768        61.8753         0.2358
   4  MOLE-FLOW        S1       MIXED    DPC
LBMOL/HR       60.1147        60.1146      9.3750-03
   5  MOLE-FLOW        S1       MIXED    CO
LBMOL/HR      567.5629       567.5103         0.9282
   6  MOLE-FLOW        S1       MIXED    O2
LBMOL/HR        0.0            0.0            0.0
   7  MOLE-FLOW        S1       MIXED    PALLA-01
LBMOL/HR        0.3645         0.3645     -6.7216-05
   8  PRESSURE         S1       MIXED
PSIA          145.0377       145.0377         0.0
```

```
   9  MASS ENTHALPY    S1        MIXED
BTU/LB       -845.3608      -845.3484        -0.1471

                          *** ITERATION HISTORY ***

     TEAR STREAMS AND TEAR VARIABLES:

     ITERATION   MAX-ERR/TOL   STREAM ID      VARIABLE
SUBSTREA COMPONEN ATTRIBUT ELEMENT
     ---------   -----------   ---------      ---------------- -------
- -------- -------- -------
          1       319.3        S1             MOLE-FLOW        MIXED
WATER
          2       105.8        S1             MOLE-FLOW        MIXED
CO
          3       69.34        S1             MOLE-FLOW        MIXED
CO
          4      -71.67        S1             MOLE-FLOW        MIXED
WATER
          5       32.21        S1             MASS ENTHALPY    MIXED
          6      -25.86        S1             MASS ENTHALPY    MIXED
          7       13.23        S1             MOLE-FLOW        MIXED
CO
          8       8.951        S1             MOLE-FLOW        MIXED
CO
          9       6.090        S1             MOLE-FLOW        MIXED
CO
         10      -6.622        S1             MOLE-FLOW        MIXED
WATER
         11       6.173        S1             MASS ENTHALPY    MIXED
         12      -3.141        S1             MASS ENTHALPY    MIXED
         13       1.346        S1             MOLE-FLOW        MIXED
CO
         14      0.9282        S1             MOLE-FLOW        MIXED
CO
```

```
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                                FLOWSHEET SECTION

 COMPUTATIONAL SEQUENCE
 ----------------------

 SEQUENCE USED WAS:
    *$OLVER01 F1 C1 S1 V1 F2 COM1 D1 C2 F3 P2 D2 P3 C4 S2 P1 R1
    (RETURN *$OLVER01)
    P4 C3

 OVERALL FLOWSHEET BALANCE
 -------------------------

                       ***  MASS AND ENERGY BALANCE  ***
                                  IN          OUT       GENERATION
RELATIVE DIFF.
   CONVENTIONAL COMPONENTS
            (LBMOL/HR)
      PHENOL              122.220       3.16554      -119.050
0.361809E-04
      WATER               0.00000       59.5234       59.5248
0.245072E-04
      DPC                 0.00000       59.5248       59.5248
0.946443E-06
      CO                  105.128       45.5505      -59.5248
0.501093E-03
      O2                  29.7624       0.00000      -29.7624
0.00000
      PALLA-01           0.364512E-02  0.364512E-02   0.00000
0.118186E-06
   TOTAL BALANCE
   MOLE(LBMOL/HR)         257.114       167.768      -89.2872
0.227977E-03
   MASS(LB/HR   )         15400.1       15397.6
0.166300E-03
   ENTHALPY(BTU/HR  )   -0.124749E+08 -0.201924E+08
0.382198

                       ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
PHENOL	C	C6H6O	PHENOL
WATER	C	H2O	WATER
DPC	C	MISSING	MISSING
CO	C	CO	CARBON-MONOXIDE
O2	C	O2	OXYGEN
PALLA-01	C	PDCL2	PALLADIUM-CHLORIDE

LISTID	SUPERCRITICAL COMPONENT LIST
CO	CO
O2	O2

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  C1       MODEL: HEATER
 ------------------------------
   INLET STREAM:          S2
   OUTLET STREAM:         S3
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
   DIRTY WATER OPTION SET: SYSOP12   ASME STEAM TABLE
   SOLUBLE WATER OPTION:  THE MAIN PROPERTY OPTION SET (NRTL    ).

                       ***  MASS AND ENERGY BALANCE  ***
                                     IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            552.703         552.703
0.00000
       MASS(LB/HR   )            15522.8         15522.8
0.00000
       ENTHALPY(BTU/HR  )      -0.260045E+08   -0.264304E+08
0.161153E-01

                       ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                           ***  INPUT DATA  ***
   THREE  PHASE  TP  FLASH
   DIRTY WATER CONSIDERED
   SPECIFIED TEMPERATURE               F
77.0000
   SPECIFIED PRESSURE                  PSIA
145.038
   MAXIMUM NO. ITERATIONS                                        30
   CONVERGENCE TOLERANCE
0.000100000



                             ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     77.000
   OUTLET PRESSURE       PSIA                                  145.04
   HEAT DUTY             BTU/HR                             -
0.42593E+06
   OUTLET VAPOR FRACTION                                     0.99640
   OUTLET: 1ST LIQUID/TOTAL LIQUID                            1.0000
   PRESSURE-DROP CORRELATION PARAMETER                        0.0000
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  C1       MODEL: HEATER (CONTINUED)

   V-L1-L2 PHASE EQUILIBRIUM :

      COMP           F(I)      X1(I)     X2(I)     Y(I)      K1(I)
K2(I)
      PHENOL        0.176E-02 0.481     0.481     0.292E-04 0.607E-04
0.607E-04
      WATER         0.416E-02 0.494     0.494     0.239E-02 0.483E-02
0.483E-02
      DPC           0.347E-08 0.962E-06 0.962E-06 0.767E-15 0.797E-09
0.797E-09
      CO            0.994     0.257E-01 0.257E-01 0.998      38.8
38.8

 BLOCK:  C2       MODEL: HEATER
 ------------------------------
   INLET STREAM:          S12
   OUTLET STREAM:         S13
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1253.05          1253.05
0.00000
       MASS(LB/HR   )            112200.          112200.
0.259392E-15
       ENTHALPY(BTU/HR  )      -0.520288E+08   -0.859975E+08
0.394997

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE               F
77.0000
   SPECIFIED PRESSURE                  PSIA
0.48342
   MAXIMUM NO. ITERATIONS                                        30
```

```
   CONVERGENCE TOLERANCE
0.000100000
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  C2       MODEL: HEATER (CONTINUED)

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    77.000
   OUTLET PRESSURE       PSIA                                0.48342
   HEAT DUTY             BTU/HR                             -
0.33969E+08
   OUTLET VAPOR FRACTION                                     0.15735E-
01
   PRESSURE-DROP CORRELATION PARAMETER                        0.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)
K(I)
      PHENOL           0.93803        0.95276        0.16474E-01
0.17291E-01
      WATER            0.47545E-01    0.47146E-01    0.72502E-01
1.5378
      CO               0.14428E-01    0.94845E-04    0.91102
9605.4

 BLOCK:  C3       MODEL: HEATER
 ------------------------------
   INLET STREAM:          S20
   OUTLET STREAM:         FINALDPC
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            62.1850         62.1850
0.00000
       MASS(LB/HR   )            13000.4         13000.4
0.00000
       ENTHALPY(BTU/HR  )      -0.107889E+08   -0.118796E+08
0.918160E-01

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
                          ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE               F
212.000
   PRESSURE DROP                       PSI
5.00000
   MAXIMUM NO. ITERATIONS                                          30
   CONVERGENCE TOLERANCE
0.000100000
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  C3       MODEL: HEATER (CONTINUED)

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    212.00
   OUTLET PRESSURE       PSIA                                 14.500
   HEAT DUTY             BTU/HR                            -
0.10907E+07
   OUTLET VAPOR FRACTION                                      0.0000
   PRESSURE-DROP CORRELATION PARAMETER
0.14502E+08



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)
K(I)
      PHENOL          0.42875E-01    0.42875E-01    0.27496
0.40059E-02
      DPC             0.95712        0.95712        0.72504
0.47318E-03

 BLOCK:  C4       MODEL: HEATER
 ------------------------------
   INLET STREAM:          S17
   OUTLET STREAM:         S18
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1175.12          1175.12
0.00000
       MASS(LB/HR   )            110581.          110581.
0.00000
       ENTHALPY(BTU/HR  )      -0.606308E+08   -0.718916E+08
0.156635

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          ***  INPUT DATA  ***
```

```
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE                F
194.000
   SPECIFIED PRESSURE                   PSIA
145.038
   MAXIMUM NO. ITERATIONS                                        30
   CONVERGENCE TOLERANCE
0.000100000
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  C4       MODEL: HEATER (CONTINUED)

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    194.00
   OUTLET PRESSURE       PSIA                                 145.04
   HEAT DUTY             BTU/HR                             -
0.11261E+08
   OUTLET VAPOR FRACTION                                      0.0000
   PRESSURE-DROP CORRELATION PARAMETER                        0.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)
K(I)
      PHENOL           0.99986        0.99986        0.99474
0.34044E-02
      WATER            0.14347E-03    0.14347E-03    0.52593E-02
0.12544
      CO               0.27428E-13    0.27428E-13    0.49127E-09
61.292

 BLOCK:  COM1     MODEL: COMPR
 ------------------------------
   INLET STREAM:          S10
   OUTLET STREAM:         S11
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1315.24          1315.24
0.00000
       MASS(LB/HR   )            125200.          125200.
0.232458E-15
       ENTHALPY(BTU/HR  )      -0.596879E+08   -0.533506E+08   -
0.106173

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

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 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  COM1     MODEL: COMPR (CONTINUED)

                            ***  INPUT DATA  ***

   ISENTROPIC CENTRIFUGAL COMPRESSOR
    OUTLET PRESSURE  PSIA                                    1.45038
    ISENTROPIC EFFICIENCY                                    0.72000
    MECHANICAL EFFICIENCY                                    1.00000

                            ***  RESULTS  ***

    INDICATED  HORSEPOWER REQUIREMENT  HP                 2,490.64
    BRAKE      HORSEPOWER REQUIREMENT  HP                 2,490.64
    NET WORK REQUIRED                  HP                 2,490.64
    POWER LOSSES                       HP                     0.0
    ISENTROPIC HORSEPOWER REQUIREMENT  HP                 1,793.26
    CALCULATED OUTLET TEMP  F                               387.907
    ISENTROPIC TEMPERATURE  F                               350.589
    EFFICIENCY (POLYTR/ISENTR) USED                          0.72000
    OUTLET VAPOR FRACTION                                    1.00000
    HEAD DEVELOPED,       FT-LBF/LB                     28,359.8
    MECHANICAL EFFICIENCY USED                               1.00000
    INLET HEAT CAPACITY RATIO                                1.06618
    INLET VOLUMETRIC FLOW RATE , CUFT/HR
0.688670+08
    OUTLET VOLUMETRIC FLOW RATE, CUFT/HR             8,248,200.
    INLET  COMPRESSIBILITY FACTOR                            1.00000
    OUTLET COMPRESSIBILITY FACTOR                            1.00000
    AV. ISENT. VOL. EXPONENT                                 1.06247
    AV. ISENT. TEMP EXPONENT                                 1.06247
    AV. ACTUAL VOL. EXPONENT                                 1.08501
    AV. ACTUAL TEMP EXPONENT                                 1.08501

 BLOCK:  D1       MODEL: RADFRAC
 ------------------------------
    INLETS   - S11      STAGE   5
    OUTLETS  - S12      STAGE   1
               S19      STAGE  14
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
```

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 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D1       MODEL: RADFRAC (CONTINUED)

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1315.24         1315.24
0.00000
       MASS(LB/HR   )            125200.         125200.       -
0.929831E-15
       ENTHALPY(BTU/HR  )      -0.533506E+08   -0.628197E+08
0.150733

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR



                         **********************
                         ****  INPUT DATA  ****
                         **********************

   ****   INPUT PARAMETERS   ****

    NUMBER OF STAGES                                        14
    ALGORITHM OPTION                                    NONIDEAL
    ABSORBER OPTION                                     NO
    INITIALIZATION OPTION                               STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                    NO
    INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
    DESIGN SPECIFICATION METHOD                         NESTED
    MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS               100
    MAXIMUM NO. OF INSIDE LOOP ITERATIONS                 10
    MAXIMUM NUMBER OF FLASH ITERATIONS                    30
    FLASH TOLERANCE
0.000100000
    OUTSIDE LOOP CONVERGENCE TOLERANCE
0.000100000

   ****   COL-SPECS   ****

    MOLAR VAPOR DIST / TOTAL DIST                        1.00000
    MOLAR REFLUX RATIO                                   0.65125
```

MOLAR BOILUP RATIO	6.43259

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D1       MODEL: RADFRAC (CONTINUED)

   ****    PROFILES   ****

    P-SPEC          STAGE   1  PRES, PSIA                    0.48342

                         ********************
                         ****  RESULTS  ****
                         ********************


   ***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
                 S12          S19
    COMPONENT:
    PHENOL      .99774       .22632E-02
    WATER      1.0000        0.0000
    DPC        0.0000        1.0000
    CO         1.0000        0.0000


   ***    SUMMARY OF KEY RESULTS    ***

    TOP STAGE TEMPERATURE          F                        190.950
    BOTTOM STAGE TEMPERATURE       F                        401.393
    TOP STAGE LIQUID FLOW          LBMOL/HR                 816.051
    BOTTOM STAGE LIQUID FLOW       LBMOL/HR                  62.1850
    TOP STAGE VAPOR FLOW           LBMOL/HR               1,253.05
    BOILUP VAPOR FLOW              LBMOL/HR                 400.010
    MOLAR REFLUX RATIO                                        0.65125
    MOLAR BOILUP RATIO                                        6.43259
    CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                    -
0.204173+08
    REBOILER DUTY                  BTU/HR
0.109483+08

   ****   MAXIMUM FINAL RELATIVE ERRORS   ****

    DEW POINT                       0.53010E-04  STAGE= 11
    BUBBLE POINT                    0.26017E-03  STAGE= 10
    COMPONENT MASS BALANCE          0.12324E-04  STAGE=  9 COMP=DPC
    ENERGY BALANCE                  0.62631E-04  STAGE= 10
```

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U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	190.95	0.48342	-61391.	-41522.	-.20417+08
2	218.32	0.96684	-60088.	-39490.	
3	218.91	0.98024	-60070.	-39421.	
4	231.11	0.99324	-75394.	-39088.	
5	233.07	1.0045	-75184.	-37088.	
10	302.65	1.0077	-0.11434E+06	-37450.	
11	373.26	1.0085	-0.14608E+06	-75191.	
12	393.28	1.0097	-0.16153E+06	-0.11432E+06	
13	399.08	1.0110	-0.16930E+06	-0.13249E+06	
14	401.39	1.0124	-0.17353E+06	-0.14127E+06	.10948+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	816.1	1253.					1253.0544
2	860.6	2069.					
3	827.7	2114.					
4	507.3	2081.			1315.2394		
5	509.6	445.1					
10	435.8	406.6					
11	460.6	373.7					
12	464.9	398.4					
13	462.2	402.7					
14	62.19	400.0				62.1850	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	

```
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1 0.7672E+05 0.1122E+06
.11220+06
   2 0.8093E+05 0.1889E+06
   3 0.7785E+05 0.1931E+06
   4 0.5487E+05 0.1900E+06           .12520+06
   5 0.5511E+05 0.4187E+05
  10 0.6406E+05 0.3933E+05
  11 0.8342E+05 0.5106E+05
  12 0.9165E+05 0.7042E+05
  13 0.9470E+05 0.7865E+05
  14 0.1300E+05 0.8170E+05                                  .13000+05
```

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U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

**** MOLE-X-PROFILE ****

STAGE	PHENOL	WATER	DPC	CO
1	0.99865	0.13503E-02	0.95883E-13	0.79571E-06
2	0.99906	0.93984E-03	0.29225E-08	0.85096E-06
3	0.99899	0.91713E-03	0.91070E-04	0.84194E-06
4	0.88204	0.60307E-03	0.11736	0.52068E-06
5	0.88315	0.13930E-04	0.11684	0.35716E-10
10	0.55975	0.16415E-13	0.44025	0.29839E-31
11	0.27566	0.17250E-16	0.72434	0.10459E-35
12	0.14217	0.97597E-20	0.85783	0.35100E-40
13	0.77520E-01	0.41539E-23	0.92248	0.11624E-44
14	0.42875E-01	0.15168E-26	0.95712	0.38300E-49

**** MOLE-Y-PROFILE ****

STAGE	PHENOL	WATER	DPC	CO
1	0.93803	0.47545E-01	0.91246E-18	0.14428E-01
2	0.96194	0.29326E-01	0.37817E-13	0.87379E-02
3	0.96288	0.28569E-01	0.11899E-08	0.85537E-02
4	0.96228	0.28997E-01	0.36226E-04	0.86890E-02
5	0.99927	0.68732E-03	0.37625E-04	0.59342E-06
10	0.97836	0.40148E-11	0.21635E-01	0.83971E-27
11	0.64577	0.19147E-13	0.35423	0.34805E-31
12	0.31199	0.19942E-16	0.68801	0.12091E-35
13	0.15750	0.11267E-19	0.84250	0.40520E-40
14	0.82905E-01	0.47994E-23	0.91709	0.13431E-44

**** K-VALUES ****

STAGE	PHENOL	WATER	DPC	CO
1	0.93930	35.210	0.95164E-05	18132.
2	0.96284	31.204	0.12940E-04	10268.
3	0.96385	31.151	0.13066E-04	10159.
4	1.0910	48.083	0.30868E-03	16688.
5	1.1315	49.342	0.32203E-03	16615.
10	1.7483	244.53	0.49128E-01	28138.
11	2.3425	1109.9	0.48901	33284.
12	2.1944	2043.2	0.80204	34447.
13	2.0316	2712.3	0.91329	34859.
14	1.9335	3164.0	0.95818	35068.

**** MASS-X-PROFILE ****

STAGE	PHENOL	WATER	DPC	CO
1	0.99974	0.25877E-03	0.21848E-12	0.23708E-06
2	0.99982	0.18004E-03	0.66568E-08	0.25346E-06
3	0.99962	0.17567E-03	0.20741E-03	0.25074E-06
4	0.76748	0.10045E-03	0.23242	0.13484E-06

5	0.76857	0.23205E-05	0.23143	0.92508E-11
10	0.35840	0.20119E-14	0.64160	0.56863E-32
11	0.14325	0.17159E-17	0.85675	0.16176E-36
12	0.67871E-01	0.89189E-21	0.93213	0.49872E-41
13	0.35606E-01	0.36522E-24	0.96439	0.15890E-45
14	0.19301E-01	0.13071E-27	0.98070	0.51315E-50

U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

**** MASS-Y-PROFILE ****

STAGE	PHENOL	WATER	DPC	CO
1	0.98592	0.95659E-02	0.21829E-17	0.45134E-02
2	0.99153	0.57864E-02	0.88722E-13	0.26806E-02
3	0.99175	0.56327E-02	0.27896E-08	0.26221E-02
4	0.99153	0.57195E-02	0.84961E-04	0.26647E-02
5	0.99978	0.13164E-03	0.85682E-04	0.17671E-06
10	0.95208	0.74788E-12	0.47921E-01	0.24320E-27
11	0.44473	0.25241E-14	0.55527	0.71340E-32
12	0.16613	0.20327E-17	0.83387	0.19162E-36
13	0.75900E-01	0.10393E-20	0.92410	0.58116E-41
14	0.38200E-01	0.42331E-24	0.96180	0.18419E-45

****
***** HYDRAULIC PARAMETERS *****
****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

STAGE	TEMPERATURE F LIQUID FROM	TEMPERATURE F VAPOR TO
1	190.95	218.32
2	218.32	218.91
3	218.91	231.11
4	231.11	351.04
5	233.07	233.12

10	302.65	373.26
11	373.26	393.28
12	393.28	399.08
13	399.08	401.39
14	401.39	401.39

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U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

	MASS FLOW		VOLUME FLOW		MOLECULAR WEIGHT	
	LB/HR		CUFT/HR			
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	76717.	0.18892E+06	1200.0	0.15571E+08	94.010	91.304
2	80934.	0.19313E+06	1283.7	0.15702E+08	94.041	91.374
3	77848.	0.19005E+06	1235.1	0.15530E+08	94.054	91.336
4	54871.	0.16707E+06	877.63	0.15419E+08	108.16	94.907
5	55106.	42106.	882.36	0.33092E+07	108.14	94.116
10	64063.	51063.	1019.8	0.33118E+07	146.99	136.66
11	83421.	70421.	1295.4	0.36121E+07	181.10	176.74
12	91648.	78647.	1391.3	0.36708E+07	197.14	195.29
13	94704.	81703.	1417.9	0.36511E+07	204.90	204.25
14	13000.	0.0000	193.09	0.0000	209.06	

	DENSITY		VISCOSITY		SURFACE TENSION
	LB/CUFT		CP		DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	63.930	0.12133E-01	1.2444	0.92049E-02	33.790
2	63.048	0.12300E-01	0.86126	0.92095E-02	32.120
3	63.028	0.12238E-01	0.85479	0.93792E-02	32.083
4	62.521	0.10835E-01	0.85811	0.10912E-01	31.199
5	62.453	0.12724E-01	0.83799	0.92611E-02	31.071
10	62.820	0.15418E-01	0.64167	0.99852E-02	27.000
11	64.398	0.19496E-01	0.57423	0.93296E-02	23.560
12	65.874	0.21425E-01	0.63067	0.90334E-02	22.764
13	66.791	0.22378E-01	0.68034	0.88949E-02	22.584
14	67.328		0.71255		22.527

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.55944E-02	0.21453E+06	0.17151E+07
2	-1.6697	0.58531E-02	0.21934E+06	0.17415E+07
3	-.36754E-01	0.57078E-02	0.21642E+06	0.17180E+07
4	-.88448	0.43236E-02	0.20301E+06	0.16050E+07
5	-.12835	0.18681E-01	47239.	0.37328E+06
10	-3.7680	0.19655E-01	51891.	0.41123E+06
11	-3.4408	0.20611E-01	62858.	0.50435E+06
12	-.79569	0.21016E-01	66212.	0.53731E+06
13	-.17989	0.21217E-01	66841.	0.54617E+06
14	-.56491E-01		0.0000	0.0000

U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

****
***** PACKING SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		13
CAPACITY CALCULATION METHOD		SULZER
PRESSURE DROP CALCULATION METHOD		SULZER
LIQUID HOLDUP CALCULATION METHOD		STICHL
PRESSURE PROFILE UPDATED		YES

DESIGN PARAMETERS

OVERDESIGN FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FRAC. APP. TO MAXIMUM CAPACITY		0.62000
MAXIMUM CAPACITY FACTOR	FT/SEC	MISSING
DESIGN CAPACITY FACTOR	FT/SEC	MISSING
PRESSURE DROP FOR THE SECTION	PSI	MISSING
PRESSURE DROP PER UNIT HEIGHT	IN-WATER/FT	MISSING

PACKING SPECIFICATIONS

PACKING TYPE		MELLAPAK
PACKING MATERIAL		STANDARD
PACKING SIZE		125X
VENDOR		SULZER
PACKING FACTOR	1/FT	MISSING
PACKING SURFACE AREA	SQFT/CUF	35.3572
PACKING VOID FRACTION		0.98800
FIRST STICHLMAIR CONSTANT		1.00000
SECOND STICHLMAIR CONSTANT		1.00000
THIRD STICHLMAIR CONSTANT		0.32000
HETP	FT	1.41667
PACKING HEIGHT	FT	17.0000
PACKING SHEET THICKNESS	FT	0.00065617

***** SIZING RESULTS *****

COLUMN DIAMETER	FT	11.6652
MAXIMUM FRACTIONAL CAPACITY		0.62000
MAXIMUM CAPACITY FACTOR	FT/SEC	0.57009
PRESSURE DROP FOR THE SECTION	PSI	0.045537
AVERAGE PRESSURE DROP/HEIGHT	IN-WATER/FT	0.074144
MAXIMUM LIQUID HOLDUP/STAGE	CUFT	2.42444
MAX LIQ SUPERFICIAL VELOCITY	FT/SEC	0.0036853

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U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

**** RATING PROFILES AT MAXIMUM COLUMN DIAMETER ****

STAGE	HEIGHT FROM TOP OF SECTION FT	FRACTIONAL CAPACITY	PRESSURE DROP PSI	PRESSURE DROP/HEIGHT IN-WATER/FT	LIQUID HOLDUP CUFT	HETP FT
2	0.000	0.6200	0.13405E-01	0.26191	2.424	1.417
3	1.417	0.6092	0.12995E-01	0.25390	2.396	1.417
4	2.833	0.5483	0.11223E-01	0.21928	2.224	1.417
5	4.250	0.1725	0.65709E-03	0.12839E-01	2.163	1.417
6	5.667	0.1725	0.65684E-03	0.12834E-01	2.163	1.417
7	7.083	0.1725	0.65643E-03	0.12826E-01	2.163	1.417
8	8.500	0.1719	0.65301E-03	0.12759E-01	2.161	1.417
9	9.917	0.1661	0.61926E-03	0.12100E-01	2.133	1.417
10	11.33	0.1952	0.79478E-03	0.15529E-01	2.083	1.417
11	12.75	0.2371	0.11762E-02	0.22981E-01	2.125	1.417
12	14.17	0.2511	0.13293E-02	0.25972E-01	2.201	1.417
13	15.58	0.2541	0.13718E-02	0.26803E-01	2.246	1.417

STAGE	LIQUID SUPERFICIAL VELOCITY FT/SEC
2	0.3336E-02
3	0.3210E-02
4	0.2281E-02
5	0.2293E-02
6	0.2294E-02
7	0.2293E-02
8	0.2283E-02

```
  9   0.2180E-02
 10   0.2651E-02
 11   0.3367E-02
 12   0.3616E-02
 13   0.3685E-02
```

U-O-S BLOCK SECTION

BLOCK: D1 MODEL: RADFRAC (CONTINUED)

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		13
FLOODING CALCULATION METHOD		B960

DESIGN PARAMETERS

PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		FLEXI
NUMBER OF PASSES		1
TRAY SPACING	FT	2.00000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		2
COLUMN DIAMETER	FT	15.3586
DC AREA/COLUMN AREA		0.10000
DOWNCOMER VELOCITY	FT/SEC	0.019247
FLOW PATH LENGTH	FT	10.5521
SIDE DOWNCOMER WIDTH	FT	2.40325
SIDE WEIR LENGTH	FT	11.1598
CENTER DOWNCOMER WIDTH	FT	0.0
CENTER WEIR LENGTH	FT	0.0
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	0.0
OFF-CENTER LONG WEIR LENGTH	FT	0.0
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER FT	TOTAL AREA SQFT	ACTIVE AREA SQFT	SIDE DC AREA SQFT
2	15.359	185.27	148.21	18.527
3	15.239	182.39	145.91	18.239
4	14.625	168.00	134.40	16.800
5	7.2498	41.280	33.024	4.1280
6	7.2492	41.273	33.019	4.1273
7	7.2481	41.260	33.008	4.1260
8	7.2361	41.124	32.900	4.1124
9	7.1120	39.726	31.781	3.9726
10	7.6393	45.835	36.668	4.5835
11	8.4829	56.518	45.214	5.6518
12	8.7333	59.902	47.922	5.9902

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D1       MODEL: RADFRAC (CONTINUED)

       STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
                  FT            SQFT         SQFT           SQFT
         13       8.7834        60.592       48.474        6.0592

 BLOCK:  D2       MODEL: RADFRAC
 ------------------------------
    INLETS   - S15      STAGE   8
    OUTLETS  - H2O      STAGE   1
               S16      STAGE  11
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1233.34         1233.34
0.00000
       MASS(LB/HR   )            111641.         111641.       -
0.378004E-14
       ENTHALPY(BTU/HR  )      -0.849722E+08   -0.666752E+08   -
0.215329

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

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 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D2       MODEL: RADFRAC (CONTINUED)


                         **********************
                         ****  INPUT DATA  ****
                         **********************

   ****   INPUT PARAMETERS   ****

    NUMBER OF STAGES                                          11
    ALGORITHM OPTION                                      STANDARD
    ABSORBER OPTION                                       NO
    INITIALIZATION OPTION                                 STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                      NO
    INSIDE LOOP CONVERGENCE METHOD                        BROYDEN
    DESIGN SPECIFICATION METHOD                           NESTED
    MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                100
    MAXIMUM NO. OF INSIDE LOOP ITERATIONS                  10
    MAXIMUM NUMBER OF FLASH ITERATIONS                     30
    FLASH TOLERANCE
0.000100000
    OUTSIDE LOOP CONVERGENCE TOLERANCE
0.000100000

   ****   COL-SPECS   ****

    MOLAR VAPOR DIST / TOTAL DIST                          1.00000
    MOLAR REFLUX RATIO                                     1.02445
    MOLAR BOILUP RATIO                                     0.83150

   ****    PROFILES   ****

    P-SPEC          STAGE   1  PRES, PSIA                  14.5038

                         ********************
                         ****  RESULTS  ****
                         ********************


   ***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
                 H2O          S16
    COMPONENT:
    PHENOL      .10367E-03   .99990
```

WATER	.99710	.28993E-02
CO	1.0000	.27554E-09

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D2       MODEL: RADFRAC (CONTINUED)


   ***    SUMMARY OF KEY RESULTS    ***

    TOP STAGE TEMPERATURE          F                        211.448
    BOTTOM STAGE TEMPERATURE       F                        379.656
    TOP STAGE LIQUID FLOW          LBMOL/HR                  59.6414
    BOTTOM STAGE LIQUID FLOW       LBMOL/HR               1,175.12
    TOP STAGE VAPOR FLOW           LBMOL/HR                  58.2178
    BOILUP VAPOR FLOW              LBMOL/HR                 977.108
    MOLAR REFLUX RATIO                                        1.02445
    MOLAR BOILUP RATIO                                        0.83150
    CONDENSER DUTY (W/O SUBCOOL)   BTU/HR           -1,059,790.
    REBOILER DUTY                  BTU/HR
0.193568+08

   ****   MAXIMUM FINAL RELATIVE ERRORS   ****

    DEW POINT                       0.26594E-03  STAGE=  6
    BUBBLE POINT                    0.31500E-03  STAGE=  6
    COMPONENT MASS BALANCE          0.10636E-05  STAGE=  6 COMP=CO
    ENERGY BALANCE                  0.53425E-04  STAGE=  7


   ****    PROFILES   ****

   **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE
FLOWS
            FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                                          ENTHALPY
 STAGE TEMPERATURE   PRESSURE             BTU/LBMOL           HEAT DUTY
       F             PSIA           LIQUID       VAPOR        BTU/HR

   1   211.45        14.504      -0.12006E+06 -0.10263E+06  -.10598+07
   2   223.82        18.371      -0.11948E+06 -0.10246E+06
   6   249.72        19.029       -81414.      -98088.
   7   305.84        19.193       -62206.      -83076.
   8   324.58        19.357       -58828.      -74431.
   9   366.79        19.522       -53047.      -44155.
  10   377.68        19.686       -51841.      -33781.
  11   379.66        19.850       -51655.      -32255.       .19357+08
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  D2       MODEL: RADFRAC (CONTINUED)

 STAGE     FLOW RATE                   FEED RATE                PRODUCT
RATE
            LBMOL/HR                    LBMOL/HR
LBMOL/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1  59.64      58.22
58.2177
   2  60.38      117.9
   6  47.17      115.7
   7  47.59      105.4
   8  1920.      105.8      1233.3381
   9  2095.      744.7
  10  2152.      919.8
  11  1175.      977.1                                    1175.1204

    ****  MASS FLOW PROFILES  ****

 STAGE     FLOW RATE                   FEED RATE                PRODUCT
RATE
            LB/HR                       LB/HR                    LB/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1  1101.      1059.
1059.2490
   2  1139.      2160.
   6  3096.      2675.
   7  4102.      4155.
   8 0.1711E+06  5162.      .11164+06
   9 0.1955E+06 0.6055E+05
  10 0.2023E+06 0.8491E+05
  11 0.1106E+06 0.9176E+05                                 .11058+06

                          ****   MOLE-X-PROFILE     ****
   STAGE     PHENOL         WATER          CO
      1    0.58375E-02   0.99416       0.11872E-05
      2    0.11232E-01   0.98877       0.73569E-06
      6    0.62578       0.37422       0.16030E-05
      7    0.89617       0.10383       0.15098E-05
      8    0.93465       0.65349E-01   0.14341E-05
      9    0.98955       0.10454E-01   0.42728E-08
     10    0.99871       0.12903E-02   0.11000E-10
     11    0.99986       0.14347E-03   0.27428E-13

                          ****   MOLE-Y-PROFILE     ****
```

STAGE	PHENOL	WATER	CO
1	0.20925E-02	0.99590	0.20093E-02
2	0.39876E-02	0.99502	0.99311E-03
6	0.66908E-01	0.93208	0.10114E-02
7	0.28123	0.71766	0.11107E-02
8	0.40421	0.59468	0.11063E-02
9	0.83175	0.16825	0.36973E-05
10	0.97637	0.23627E-01	0.97316E-08
11	0.99733	0.26696E-02	0.24197E-10

U-O-S BLOCK SECTION

BLOCK: D2 MODEL: RADFRAC (CONTINUED)

**** K-VALUES ****

STAGE	PHENOL	WATER	CO
1	0.35846	1.0017	1692.4
2	0.35499	1.0063	1349.8
6	0.10694	2.4915	629.76
7	0.31384	6.9108	734.90
8	0.43247	9.0997	771.23
9	0.84054	16.093	865.24
10	0.97763	18.311	884.66
11	0.99747	18.608	882.20

**** MASS-X-PROFILE ****

STAGE	PHENOL	WATER	CO
1	0.29762E-01	0.97024	0.18015E-05
2	0.56020E-01	0.94398	0.10921E-05
6	0.89729	0.10271	0.68407E-06
7	0.97830	0.21697E-01	0.49053E-06
8	0.98679	0.13207E-01	0.45065E-06
9	0.99798	0.20183E-02	0.12825E-08
10	0.99975	0.24725E-03	0.32774E-11
11	0.99997	0.27466E-04	0.81643E-14

**** MASS-Y-PROFILE ****

STAGE	PHENOL	WATER	CO
1	0.10824E-01	0.98608	0.30933E-02
2	0.20476E-01	0.97801	0.15177E-02
6	0.27239	0.72638	0.12254E-02
7	0.67129	0.32792	0.78910E-03
8	0.77976	0.21960	0.63517E-03
9	0.96272	0.37277E-01	0.12737E-05
10	0.99539	0.46108E-02	0.29528E-08
11	0.99949	0.51213E-03	0.72173E-11

U-O-S BLOCK SECTION

BLOCK: D2 MODEL: RADFRAC (CONTINUED)

****
***** HYDRAULIC PARAMETERS *****
****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

	TEMPERATURE F	
STAGE	LIQUID FROM	VAPOR TO
1	211.45	223.82
2	223.82	224.57
6	249.72	305.84
7	305.84	324.58
8	324.58	366.79
9	366.79	377.68
10	377.68	379.66
11	379.66	379.66

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	1101.0	2160.2	19.093	47056.	18.460	18.329
2	1139.3	2198.6	19.821	46981.	18.870	18.538

```
    6   3095.7      4155.0      48.125      45106.      65.636
39.427
    7   4102.5      5161.7      67.443      46001.      86.212
48.786
    8  0.17113E+06  60549.      2857.0     0.33832E+06  89.140
81.310
    9  0.19549E+06  84913.      3370.9     0.41986E+06  93.317
92.315
   10  0.20234E+06  91760.      3517.2     0.44336E+06  94.015
93.910
   11  0.11058E+06  0.0000      1924.9      0.0000      94.102
```

U-O-S BLOCK SECTION

BLOCK: D2 MODEL: RADFRAC (CONTINUED)

	DENSITY		VISCOSITY		SURFACE TENSION
	LB/CUFT		CP		DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	57.662	0.45907E-01	0.28243	0.12837E-01	58.157
2	57.480	0.46797E-01	0.26395	0.12852E-01	56.692
6	64.326	0.92115E-01	0.41025	0.13534E-01	39.168
7	60.829	0.11221	0.29791	0.13226E-01	29.025
8	59.899	0.17897	0.25502	0.11752E-01	27.030
9	57.994	0.20224	0.17812	0.11279E-01	23.402
10	57.530	0.20696	0.16255	0.11220E-01	22.598
11	57.449		0.15989		22.462

	MARANGONI INDEX	FLOW PARAM	QR	REDUCED F-FACTOR
STAGE	DYNE/CM		CUFT/HR	(LB-CUFT)**.5/HR
1		0.14380E-01	1328.3	10082.
2	-1.4648	0.14786E-01	1341.1	10163.
6	-14.040	0.28194E-01	1708.1	13690.
7	-10.143	0.34136E-01	1977.5	15409.
8	-14.641	0.15449	18521.	0.14313E+06
9	-3.6281	0.13596	24837.	0.18882E+06
10	-.80423	0.13226	26641.	0.20170E+06
11	-.13599		0.0000	0.0000

****
***** PACKING SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER	2
ENDING STAGE NUMBER	10
CAPACITY CALCULATION METHOD	SULZER
PRESSURE DROP CALCULATION METHOD	SULZER

LIQUID HOLDUP CALCULATION METHOD		STICHL
PRESSURE PROFILE UPDATED		NO
DESIGN PARAMETERS		

OVERDESIGN FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FRAC. APP. TO MAXIMUM CAPACITY		0.62000
MAXIMUM CAPACITY FACTOR	FT/SEC	MISSING
DESIGN CAPACITY FACTOR	FT/SEC	MISSING
PRESSURE DROP FOR THE SECTION	PSI	MISSING
PRESSURE DROP PER UNIT HEIGHT	IN-WATER/FT	MISSING

U-O-S BLOCK SECTION

BLOCK: D2 MODEL: RADFRAC (CONTINUED)

PACKING SPECIFICATIONS

PACKING TYPE		MELLAPAK
PACKING MATERIAL		STANDARD
PACKING SIZE		125X
VENDOR		SULZER
PACKING FACTOR	1/FT	MISSING
PACKING SURFACE AREA	SQFT/CUF	35.3572
PACKING VOID FRACTION		0.98800
FIRST STICHLMAIR CONSTANT		1.00000
SECOND STICHLMAIR CONSTANT		1.00000
THIRD STICHLMAIR CONSTANT		0.32000
HETP	FT	1.16667
PACKING HEIGHT	FT	10.5000
PACKING SHEET THICKNESS	FT	0.00065617

***** SIZING RESULTS *****

COLUMN DIAMETER	FT	5.60337
MAXIMUM FRACTIONAL CAPACITY		0.62000
MAXIMUM CAPACITY FACTOR	FT/SEC	0.30009
PRESSURE DROP FOR THE SECTION	PSI	0.010520
AVERAGE PRESSURE DROP/HEIGHT	IN-WATER/FT	0.027733
MAXIMUM LIQUID HOLDUP/STAGE	CUFT	0.69519
MAX LIQ SUPERFICIAL VELOCITY	FT/SEC	0.039619

**** RATING PROFILES AT MAXIMUM COLUMN DIAMETER ****

STAGE	HEIGHT FROM TOP OF SECTION FT	FRACTIONAL CAPACITY	PRESSURE DROP PSI	PRESSURE DROP/HEIGHT IN-WATER/FT	LIQUID HOLDUP CUFT	HETP FT
2	0.000	0.1868E-01	0.11739E-04	0.27852E-03	0.1230	1.167
3	1.167	0.1884E-01	0.11812E-04	0.28024E-03	0.1264	1.167
4	2.333	0.1924E-01	0.12058E-04	0.28607E-03	0.1336	1.167
5	3.500	0.2104E-01	0.13420E-04	0.31841E-03	0.1636	1.167

```
   6    4.667       0.2937E-01 0.18529E-04 0.43960E-03   0.2764
1.167
   7    5.833       0.3605E-01 0.23672E-04 0.56164E-03   0.2678
1.167
   8    7.000       0.4524     0.21430E-02 0.50843E-01   0.6952
1.167
   9    8.167       0.5818     0.37851E-02 0.89805E-01   0.6893
1.167
  10    9.333       0.6200     0.45010E-02 0.10679       0.6886
1.167
```

STAGE	LIQUID SUPERFICIAL VELOCITY FT/SEC
2	0.2233E-03
3	0.2295E-03
4	0.2427E-03
5	0.2944E-03
6	0.5421E-03
7	0.7597E-03
8	0.3218E-01
9	0.3797E-01
10	0.3962E-01

U-O-S BLOCK SECTION

BLOCK: D2 MODEL: RADFRAC (CONTINUED)

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		10
FLOODING CALCULATION METHOD		B960

DESIGN PARAMETERS

PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		FLEXI
NUMBER OF PASSES		1
TRAY SPACING	FT	2.00000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		10
COLUMN DIAMETER	FT	6.79883
DC AREA/COLUMN AREA		0.10000
DOWNCOMER VELOCITY	FT/SEC	0.26911
FLOW PATH LENGTH	FT	4.67113
SIDE DOWNCOMER WIDTH	FT	1.06385
SIDE WEIR LENGTH	FT	4.94011
CENTER DOWNCOMER WIDTH	FT	0.0
CENTER WEIR LENGTH	FT	0.0
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	0.0
OFF-CENTER LONG WEIR LENGTH	FT	0.0
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER FT	TOTAL AREA SQFT	ACTIVE AREA SQFT	SIDE DC AREA SQFT
2	1.1673	1.0703	0.85620	0.10703
3	1.1683	1.0721	0.85768	0.10721
4	1.1732	1.0810	0.86483	0.10810
5	1.2019	1.1345	0.90763	0.11345
6	1.3281	1.3853	1.1082	0.13853
7	1.4355	1.6184	1.2947	0.16184
8	5.6298	24.893	19.914	2.4893
9	6.5517	33.713	26.971	3.3713
10	6.7988	36.304	29.043	3.6304

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                              U-O-S BLOCK SECTION

 BLOCK:  F1       MODEL: FLASH2
 ------------------------------
   INLET STREAM:          S1
   OUTLET VAPOR STREAM:   S2
   OUTLET LIQUID STREAM:  S5
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
   DIRTY WATER OPTION SET: SYSOP12   ASME STEAM TABLE
   SOLUBLE WATER OPTION:  THE MAIN PROPERTY OPTION SET (NRTL    ).

                      ***  MASS AND ENERGY BALANCE  ***
                                      IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1869.31         1869.31
0.00000
       MASS(LB/HR   )            140954.         140954.       -
0.259743E-09
       ENTHALPY(BTU/HR  )      -0.119155E+09   -0.119155E+09
0.387115E-05

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                         ***  INPUT DATA  ***
   THREE  PHASE  TP  FLASH
   DIRTY WATER CONSIDERED
   SPECIFIED TEMPERATURE F                                  176.000
   SPECIFIED PRESSURE    PSIA                               145.038
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE
0.000100000

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                   176.00
   OUTLET PRESSURE       PSIA                                145.04
   HEAT DUTY             BTU/HR                             -461.27
   VAPOR FRACTION                                           0.29567
   1ST LIQUID/TOTAL LIQUID                                   1.0000

   V-L1-L2 PHASE EQUILIBRIUM :

      COMP           F(I)      X1(I)     X2(I)     Y(I)      K1(I)
K2(I)
```

```
      PHENOL         0.631     0.895     0.895     0.176E-02 0.197E-02
0.197E-02
      WATER          0.331E-01 0.453E-01 0.453E-01 0.416E-02 0.919E-01
0.919E-01
      DPC            0.322E-01 0.457E-01 0.457E-01 0.347E-08 0.760E-07
0.760E-07
      CO             0.304     0.137E-01 0.137E-01 0.994      72.4
72.4
      PALLA-01       0.195E-03 0.277E-03 0.277E-03 0.515E-83 0.186E-79
0.186E-79
```

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 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  F2       MODEL: FLASH2
 ------------------------------
   INLET STREAM:          S6
   OUTLET VAPOR STREAM:   S10
   OUTLET LIQUID STREAM:  S7
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
   DIRTY WATER OPTION SET: SYSOP12   ASME STEAM TABLE
   SOLUBLE WATER OPTION:  THE MAIN PROPERTY OPTION SET (NRTL    ).

                      ***  MASS AND ENERGY BALANCE  ***
                                       IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1316.60         1316.60       -
0.172697E-15
       MASS(LB/HR   )            125431.         125431.
0.665802E-11
       ENTHALPY(BTU/HR  )      -0.931508E+08   -0.597807E+08   -
0.358238

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                         ***  INPUT DATA  ***
   THREE  PHASE  TP  FLASH
   DIRTY WATER CONSIDERED
   SPECIFIED TEMPERATURE F                                  248.000
   SPECIFIED PRESSURE    PSIA                                 0.14504
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE
0.000100000

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    248.00
   OUTLET PRESSURE       PSIA                                0.14504
   HEAT DUTY             BTU/HR
0.33370E+08
   VAPOR FRACTION                                            0.99896
   1ST LIQUID/TOTAL LIQUID                                    1.0000

   V-L1-L2 PHASE EQUILIBRIUM :
```

```
      COMP            F(I)       X1(I)      X2(I)      Y(I)       K1(I)
K2(I)
      PHENOL         0.895      0.296      0.296      0.896       3.03
3.03
      WATER          0.453E-01 0.774E-04 0.774E-04 0.453E-01  586.
586.
      DPC            0.457E-01 0.437      0.437      0.453E-01 0.104
0.104
      CO             0.137E-01 0.860E-07 0.860E-07 0.137E-01 0.160E+06
0.160E+06
      PALLA-01       0.277E-03 0.267      0.267      0.547E-77 0.205E-76
0.205E-76
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  F3       MODEL: FLASH2
 ------------------------------
   INLET STREAM:          S13
   OUTLET VAPOR STREAM:   F3TOPS
   OUTLET LIQUID STREAM:  S14
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1253.05         1253.05
0.181456E-15
       MASS(LB/HR   )            112200.         112200.       -
0.100125E-12
       ENTHALPY(BTU/HR  )      -0.859975E+08   -0.859975E+08   -
0.173274E-15

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                         ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE F                                  77.0000
   SPECIFIED PRESSURE    PSIA                               0.48342
   MAXIMUM NO. ITERATIONS                                   30
   CONVERGENCE TOLERANCE
0.000100000

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                   77.000
   OUTLET PRESSURE       PSIA                               0.48342
   HEAT DUTY             BTU/HR                              0.0000
   VAPOR FRACTION                                           0.15735E-
01



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)
K(I)
```

```
      PHENOL            0.93803         0.95276         0.16474E-01
0.17291E-01
      WATER             0.47545E-01     0.47146E-01     0.72502E-01
1.5378
      CO                0.14428E-01     0.94845E-04     0.91102
9605.4
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  P1       MODEL: PUMP
 ----------------------------
   INLET STREAM:          S8
   OUTLET STREAM:         S9
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                       ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1.35047         1.35047
0.00000
       MASS(LB/HR   )            227.956         227.956
0.00000
       ENTHALPY(BTU/HR  )       -91827.5        -91408.1       -
0.456724E-02

                       ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          ***  INPUT DATA  ***
    OUTLET PRESSURE  PSIA                                  203.053
    DRIVER EFFICIENCY                                        1.00000

    FLASH SPECIFICATIONS:
    LIQUID PHASE CALCULATION
    NO FLASH PERFORMED
    MAXIMUM NUMBER OF ITERATIONS                            30
    TOLERANCE
0.000100000

                           ***  RESULTS  ***
    VOLUMETRIC FLOW RATE  CUFT/HR                            3.30239
    PRESSURE CHANGE  PSI                                   202.908
    NPSH AVAILABLE   FT-LBF/LB                               0.0
    FLUID POWER  HP                                          0.048733
    BRAKE POWER  HP                                          0.16483
    ELECTRICITY  KW                                          0.12291
    PUMP EFFICIENCY USED                                     0.29566
    NET WORK REQUIRED  HP                                    0.16483
    HEAD DEVELOPED FT-LBF/LB                               423.292

 BLOCK:  P2       MODEL: PUMP
```

```
 ----------------------------
   INLET STREAM:          S14
   OUTLET STREAM:         S15
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  P2       MODEL: PUMP (CONTINUED)

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1233.34         1233.34
0.00000
       MASS(LB/HR   )            111641.         111641.
0.130346E-15
       ENTHALPY(BTU/HR  )      -0.849819E+08   -0.849722E+08   -
0.114088E-03

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          ***  INPUT DATA  ***
    OUTLET PRESSURE  PSIA                                  20.3053
    DRIVER EFFICIENCY                                       1.00000

    FLASH SPECIFICATIONS:
    LIQUID PHASE CALCULATION
    NO FLASH PERFORMED
    MAXIMUM NUMBER OF ITERATIONS                           30
    TOLERANCE
0.000100000

                           ***  RESULTS  ***
    VOLUMETRIC FLOW RATE  CUFT/HR                      1,645.28
    PRESSURE CHANGE  PSI                                  19.8219
    NPSH AVAILABLE   FT-LBF/LB                             0.0
    FLUID POWER  HP                                        2.37182
    BRAKE POWER  HP                                        3.81043
    ELECTRICITY  KW                                        2.84143
    PUMP EFFICIENCY USED                                   0.62245
    NET WORK REQUIRED  HP                                  3.81043
    HEAD DEVELOPED FT-LBF/LB                              42.0653

 BLOCK:  P3       MODEL: PUMP
 ------------------------------
   INLET STREAM:          S16
   OUTLET STREAM:         S17
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
```

```
                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT
RELATIVE DIFF.
```

```
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                              U-O-S BLOCK SECTION

 BLOCK:  P3       MODEL: PUMP (CONTINUED)
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1175.12         1175.12
0.00000
       MASS(LB/HR   )            110581.         110581.
0.00000
       ENTHALPY(BTU/HR  )      -0.607005E+08   -0.606308E+08   -
0.114817E-02

                       ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                           ***  INPUT DATA  ***
    OUTLET PRESSURE  PSIA                                  145.038
    DRIVER EFFICIENCY                                        1.00000

    FLASH SPECIFICATIONS:
    LIQUID PHASE CALCULATION
    NO FLASH PERFORMED
    MAXIMUM NUMBER OF ITERATIONS                              30
    TOLERANCE
0.000100000

                            ***  RESULTS  ***
    VOLUMETRIC FLOW RATE  CUFT/HR                        1,924.88
    PRESSURE CHANGE  PSI                                   125.187
    NPSH AVAILABLE   FT-LBF/LB                               0.0
    FLUID POWER  HP                                         17.5251
    BRAKE POWER  HP                                         27.3910
    ELECTRICITY  KW                                         20.4255
    PUMP EFFICIENCY USED                                     0.63981
    NET WORK REQUIRED  HP                                   27.3910
    HEAD DEVELOPED FT-LBF/LB                               313.794

 BLOCK:  P4       MODEL: PUMP
 ------------------------------
   INLET STREAM:          S19
   OUTLET STREAM:         S20
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                       ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT
RELATIVE DIFF.
```

```
    TOTAL BALANCE
       MOLE(LBMOL/HR)             62.1850          62.1850
0.00000
       MASS(LB/HR    )            13000.4          13000.4
0.00000
       ENTHALPY(BTU/HR  )      -0.107909E+08   -0.107889E+08   -
0.187527E-03
```

```
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                              U-O-S BLOCK SECTION

 BLOCK:  P4       MODEL: PUMP (CONTINUED)

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                           ***  INPUT DATA  ***
    OUTLET PRESSURE  PSIA                                  19.5000
    DRIVER EFFICIENCY                                      1.00000

    FLASH SPECIFICATIONS:
    LIQUID PHASE CALCULATION
    NO FLASH PERFORMED
    MAXIMUM NUMBER OF ITERATIONS                           30
    TOLERANCE
0.000100000

                            ***  RESULTS  ***
    VOLUMETRIC FLOW RATE  CUFT/HR                         193.091
    PRESSURE CHANGE  PSI                                   18.4876
    NPSH AVAILABLE   FT-LBF/LB                             0.0
    FLUID POWER  HP                                        0.25962
    BRAKE POWER  HP                                        0.79530
    ELECTRICITY  KW                                        0.59306
    PUMP EFFICIENCY USED                                   0.32644
    NET WORK REQUIRED  HP                                  0.79530
    HEAD DEVELOPED FT-LBF/LB                               39.5410

 BLOCK:  R1       MODEL: RSTOIC
 ------------------------------
   INLET STREAMS:         FEED        S4          S9          S18
   OUTLET STREAM:         S1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
   DIRTY WATER OPTION SET: SYSOP12   ASME STEAM TABLE
   SOLUBLE WATER OPTION:  THE MAIN PROPERTY OPTION SET (NRTL    ).

                      ***  MASS AND ENERGY BALANCE  ***
                             IN          OUT       GENERATION
RELATIVE DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         1958.65       1869.31      -89.2872
0.299267E-04
   MASS(LB/HR   )         140956.       140954.
0.181693E-04
```

```
   ENTHALPY(BTU/HR  )    -0.109567E+09 -0.119155E+09
0.804676E-01

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
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                              U-O-S BLOCK SECTION

 BLOCK:  R1       MODEL: RSTOIC (CONTINUED)

                           ***  INPUT DATA  ***
   STOICHIOMETRY MATRIX:

    REACTION #   1:
     SUBSTREAM MIXED   :
     PHENOL    -2.00    WATER      1.00    DPC        1.00    CO
-1.00
     O2       -0.500


   REACTION CONVERSION SPECS: NUMBER=    1
     REACTION #   1:
     SUBSTREAM:MIXED    KEY COMP:O2       CONV FRAC:  1.000




   THREE  PHASE  TP  FLASH
   DIRTY WATER CONSIDERED
   SPECIFIED TEMPERATURE F                                  176.000
   SPECIFIED PRESSURE    PSIA                               145.038
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE
0.000100000
   SIMULTANEOUS REACTIONS
   GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                             ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    176.00
   OUTLET PRESSURE       PSIA                                 145.04
   HEAT DUTY             BTU/HR                             -
0.95920E+07
   VAPOR FRACTION                                           0.29569
   1ST LIQUID/TOTAL LIQUID                                   1.0000

   REACTION EXTENTS:

      REACTION          REACTION
      NUMBER            EXTENT
                        LBMOL/HR
      1                  59.525

   V-L1-L2 PHASE EQUILIBRIUM :
```

```
      COMP            F(I)       X1(I)      X2(I)      Y(I)       K1(I)
K2(I)
      PHENOL         0.631      0.895      0.895      0.176E-02 0.197E-02
0.197E-02
      WATER          0.331E-01 0.453E-01 0.453E-01 0.416E-02 0.919E-01
0.919E-01
      DPC            0.322E-01 0.457E-01 0.457E-01 0.347E-08 0.760E-07
0.760E-07
      CO             0.304      0.137E-01 0.137E-01 0.994       72.4
72.4
      PALLA-01       0.195E-03 0.277E-03 0.277E-03 0.515E-83 0.186E-79
0.186E-79
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/29/2013
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                              U-O-S BLOCK SECTION

 BLOCK:  S1       MODEL: FSPLIT
 ------------------------------
   INLET STREAM:          S3
   OUTLET STREAMS:        COPURGE     S4
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                        ***  MASS AND ENERGY BALANCE  ***
                                     IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            552.703         552.703
0.00000
       MASS(LB/HR   )            15522.8         15522.8
0.117182E-15
       ENTHALPY(BTU/HR  )      -0.264304E+08   -0.264304E+08
0.00000

                        ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                           ***  INPUT DATA  ***

  FRACTION OF FLOW                STRM=COPURGE  FRAC=
0.050000

                            ***  RESULTS  ***

  STREAM= COPURGE        SPLIT=          0.050000    KEY=  0
STREAM-ORDER=   1
          S4                           0.95000           0
2

 BLOCK:  S2       MODEL: FSPLIT
 ------------------------------
   INLET STREAM:          S7
   OUTLET STREAMS:        CATPURGE    S8
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                        ***  MASS AND ENERGY BALANCE  ***
                                     IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
```

```
       MOLE(LBMOL/HR)            1.36411          1.36411
0.00000
       MASS(LB/HR    )           230.258          230.258       -
0.123434E-15
       ENTHALPY(BTU/HR  )       -92755.1         -92755.1
0.00000
```

```
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                              U-O-S BLOCK SECTION

 BLOCK:  S2       MODEL: FSPLIT (CONTINUED)

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                           ***  INPUT DATA  ***

  FRACTION OF FLOW                STRM=CATPURGE FRAC=
0.0100000

                            ***  RESULTS  ***

  STREAM= CATPURGE       SPLIT=          0.0100000   KEY=  0
STREAM-ORDER=   1
          S8                           0.99000           0
2

 BLOCK:  V1       MODEL: VALVE
 ------------------------------
   INLET STREAM:          S5
   OUTLET STREAM:         S6
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
   DIRTY WATER OPTION SET: SYSOP12   ASME STEAM TABLE
   SOLUBLE WATER OPTION:  THE MAIN PROPERTY OPTION SET (NRTL    ).

                      ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT
RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1316.60         1316.60
0.00000
       MASS(LB/HR   )            125431.         125431.
0.00000
       ENTHALPY(BTU/HR  )      -0.931508E+08   -0.931508E+08
0.00000

                      ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
                          ***  INPUT DATA  ***

    VALVE OUTLET PRESSURE     PSIA                          0.14504
    VALVE FLOW COEF CALC.                                  NO

                          FLASH SPECIFICATIONS:
    NPHASE                                                  2
    MAX NUMBER OF ITERATIONS                               30
    CONVERGENCE TOLERANCE
0.000100000
```

U-O-S BLOCK SECTION

BLOCK: V1 MODEL: VALVE (CONTINUED)

*** RESULTS ***

VALVE PRESSURE DROP	PSI	144.893

```
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                                  STREAM SECTION

 CATPURGE COPURGE F3TOPS FEED FINALDPC
 -------------------------------------

 STREAM ID                CATPURGE   COPURGE    F3TOPS     FEED
FINALDPC
 FROM :                   S2         S1         F3         ----
C3
 TO   :                   ----       ----       ----       R1         -
---

 SUBSTREAM: MIXED
 PHASE:                   LIQUID     MIXED      VAPOR      MIXED
LIQUID
 COMPONENTS: LBMOL/HR
   PHENOL              4.0369-03  4.8670-02     0.3248   122.2196
2.6662
   WATER               1.0552-06     0.1149     1.4295     0.0
9.4323-26
   DPC                 5.9580-03  9.5836-08     0.0        0.0
59.5188
   CO                  1.1733-09    27.4716    17.9620   105.1280
0.0
   O2                     0.0        0.0        0.0       29.7624
0.0
   PALLA-01            3.6451-03     0.0        0.0     3.6451-03
0.0
 COMPONENTS: MOLE FRAC
   PHENOL                 0.2959  1.7612-03  1.6474-02     0.4754
4.2875-02
   WATER               7.7352-05  4.1581-03  7.2502-02     0.0
1.5168-27
   DPC                    0.4368  3.4679-09     0.0        0.0
0.9571
   CO                  8.6014-08     0.9941     0.9110     0.4089
0.0
   O2                     0.0        0.0        0.0        0.1158
0.0
   PALLA-01               0.2672     0.0        0.0     1.4177-05
0.0
 COMPONENTS: LB/HR
   PHENOL                 0.3799     4.5805    30.5680  1.1502+04
250.9246
   WATER               1.9009-05     2.0701    25.7524     0.0
1.6993-24
   DPC                    1.2763  2.0529-05     0.0        0.0
1.2750+04
```

```
   CO                  3.2865-08   769.4895   503.1229  2944.6783
0.0
   O2                     0.0        0.0        0.0      952.3613
0.0
   PALLA-01               0.6464     0.0        0.0        0.6464
0.0
 COMPONENTS: MASS FRAC
   PHENOL                 0.1650  5.9017-03  5.4640-02     0.7469
1.9301-02
   WATER               8.2555-06  2.6672-03  4.6032-02     0.0
1.3071-28
   DPC                    0.5543  2.6450-08     0.0        0.0
0.9807
   CO                  1.4273-08     0.9914     0.8993     0.1912
0.0
   O2                     0.0        0.0        0.0     6.1841-02
0.0
   PALLA-01               0.2807     0.0        0.0     4.1972-05
0.0
 TOTAL FLOW:
   LBMOL/HR            1.3641-02    27.6351    19.7163   257.1137
62.1850
   LB/HR                  2.3026   776.1402   559.4433  1.5400+04
1.3000+04
   CUFT/HR             3.3358-02  1093.4709  2.3489+05  6433.0363
175.8757
 STATE VARIABLES:
   TEMP   F             248.0001    77.0000    77.0000   176.0000
212.0000
   PRES   PSIA            0.1450   145.0377     0.4834   145.0377
14.5000
   VFRAC                  0.0        0.9964     1.0000     0.5171
0.0
   LFRAC                  1.0000  3.6047-03     0.0        0.4829
1.0000
   SFRAC                  0.0        0.0        0.0        0.0
0.0
 ENTHALPY:
   BTU/LBMOL          -6.7997+04 -4.7820+04 -5.1511+04 -4.8519+04 -
1.9104+05
   BTU/LB              -402.8307 -1702.6821 -1815.4007  -810.0503  -
913.7846
   BTU/HR              -927.5508 -1.3215+06 -1.0156+06 -1.2475+07 -
1.1880+07
 ENTROPY:
   BTU/LBMOL-R          -59.2752    16.4662    25.2794   -28.2422  -
286.5664
   BTU/LB-R              -0.3512     0.5863     0.8909    -0.4715    -
1.3707
```

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STREAM SECTION

CATPURGE COPURGE F3TOPS FEED FINALDPC (CONTINUED)

STREAM ID	CATPURGE	COPURGE	F3TOPS	FEED	FINALDPC
DENSITY:					
LBMOL/CUFT	0.4089	2.5273-02	8.3938-05	3.9968-02	0.3536
LB/CUFT	69.0274	0.7098	2.3817-03	2.3939	73.9184
AVG MW	168.7978	28.0853	28.3747	59.8962	209.0608

```
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                                  STREAM SECTION

 H2O S1 S10 S11 S12
 ------------------

 STREAM ID               H2O         S1          S10         S11
S12
 FROM :                  D2          R1          F2          COM1
D1
 TO   :                  ----        F1          COM1        D1
C2


 MAX CONV. ERROR:         0.0      9.2824-05      0.0         0.0
0.0
 SUBSTREAM: MIXED
 PHASE:                  VAPOR       MIXED       VAPOR       VAPOR
VAPOR
 COMPONENTS: LBMOL/HR
   PHENOL                 0.1218   1179.4417   1178.0646   1178.0646
1175.3984
   WATER                 57.9790     61.8753     59.5770     59.5770
59.5770
   DPC                    0.0        60.1146     59.5188     59.5188
1.1434-15
   CO                     0.1170    567.5103     18.0790     18.0790
18.0790
   O2                     0.0         0.0         0.0         0.0
0.0
   PALLA-01               0.0         0.3645      0.0         0.0
0.0
 COMPONENTS: MOLE FRAC
   PHENOL              2.0925-03      0.6310      0.8957      0.8957
0.9380
   WATER                  0.9959   3.3101-02   4.5297-02   4.5297-02
4.7545-02
   DPC                    0.0      3.2159-02   4.5253-02   4.5253-02
9.1246-19
   CO                  2.0093-03      0.3036   1.3746-02   1.3746-02
1.4428-02
   O2                     0.0         0.0         0.0         0.0
0.0
   PALLA-01               0.0      1.9500-04      0.0         0.0
0.0
 COMPONENTS: LB/HR
   PHENOL                11.4651   1.1100+05   1.1087+05   1.1087+05
1.1062+05
   WATER               1044.5074   1114.7010   1073.2969   1073.2969
1073.2969
```

```
   DPC                    0.0     1.2877+04  1.2750+04  1.2750+04
2.4492-13
   CO                     3.2766  1.5896+04   506.3994   506.3994
506.3994
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0       64.6373     0.0        0.0
0.0
 COMPONENTS: MASS FRAC
   PHENOL              1.0824-02     0.7875     0.8855     0.8855
0.9859
   WATER                  0.9861  7.9083-03  8.5726-03  8.5726-03
9.5659-03
   DPC                    0.0     9.1357-02     0.1018     0.1018
2.1829-18
   CO                  3.0933-03     0.1128  4.0447-03  4.0447-03
4.5134-03
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0     4.5857-04     0.0        0.0
0.0
 TOTAL FLOW:
   LBMOL/HR              58.2178  1869.3064  1315.2394  1315.2394
1253.0544
   LB/HR               1059.2491  1.4095+05  1.2520+05  1.2520+05
1.1220+05
   CUFT/HR             2.8909+04  2.7947+04  6.8867+07  8.2482+06
1.8098+07
 STATE VARIABLES:
   TEMP   F             211.4477   176.0000   248.0000   387.9066
190.9497
   PRES   PSIA           14.5038   145.0377     0.1450     1.4504
0.4834
   VFRAC                  1.0000     0.2957     1.0000     1.0000
1.0000
   LFRAC                  0.0        0.7043     0.0        0.0
0.0
   SFRAC                  0.0        0.0        0.0        0.0
0.0
 ENTHALPY:
   BTU/LBMOL          -1.0263+05 -6.3743+04 -4.5382+04 -4.0563+04 -
4.1522+04
   BTU/LB             -5640.5223  -845.3484  -476.7387  -426.1217  -
463.7144
   BTU/HR             -5.9747+06 -1.1915+08 -5.9688+07 -5.3351+07 -
5.2029+07
 ENTROPY:
   BTU/LBMOL-R           -8.7175   -51.9991   -40.5357   -38.9081   -
35.7750
   BTU/LB-R              -0.4791    -0.6896    -0.4258    -0.4087    -
0.3995
```

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STREAM SECTION

H2O S1 S10 S11 S12 (CONTINUED)

STREAM ID	H2O	S1	S10	S11	S12
DENSITY:					
LBMOL/CUFT	2.0138-03	6.6888-02	1.9098-05	1.5946-04	6.9237-05
LB/CUFT	3.6641-02	5.0436	1.8180-03	1.5179-02	6.1996-03
AVG MW	18.1946	75.4042	95.1921	95.1921	89.5412

```
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                                  STREAM SECTION

 S13 S14 S15 S16 S17
 -------------------

 STREAM ID                S13         S14         S15         S16
S17
 FROM :                   C2          F3          P2          D2
P3
 TO   :                   F3          P2          D2          P3
C4

 SUBSTREAM: MIXED
 PHASE:                   MIXED       LIQUID      LIQUID      LIQUID
LIQUID
 COMPONENTS: LBMOL/HR
   PHENOL               1175.3984   1175.0736   1175.0736   1174.9518
1174.9518
   WATER                  59.5770     58.1476     58.1476      0.1686
0.1686
   DPC                  1.1434-15      0.0         0.0         0.0
0.0
   CO                     18.0790      0.1170      0.1170   3.2232-11
3.2232-11
   O2                      0.0         0.0         0.0         0.0
0.0
   PALLA-01                0.0         0.0         0.0         0.0
0.0
 COMPONENTS: MOLE FRAC
   PHENOL                  0.9380      0.9528      0.9528      0.9999
0.9999
   WATER                4.7545-02   4.7146-02   4.7146-02   1.4347-04
1.4347-04
   DPC                  9.1246-19      0.0         0.0         0.0
0.0
   CO                   1.4428-02   9.4845-05   9.4845-05   2.7428-14
2.7428-14
   O2                      0.0         0.0         0.0         0.0
0.0
   PALLA-01                0.0         0.0         0.0         0.0
0.0
 COMPONENTS: LB/HR
   PHENOL               1.1062+05   1.1059+05   1.1059+05   1.1058+05
1.1058+05
   WATER                1073.2969   1047.5446   1047.5446      3.0372
3.0372
   DPC                  2.4492-13      0.0         0.0         0.0
0.0
```

```
   CO                    506.3994     3.2766     3.2766  9.0282-10
9.0282-10
   O2                      0.0        0.0        0.0        0.0
0.0
   PALLA-01                0.0        0.0        0.0        0.0
0.0
 COMPONENTS: MASS FRAC
   PHENOL                  0.9859     0.9906     0.9906     1.0000
1.0000
   WATER                9.5659-03  9.3832-03  9.3832-03  2.7466-05
2.7466-05
   DPC                  2.1829-18     0.0        0.0        0.0
0.0
   CO                   4.5134-03  2.9349-05  2.9349-05  8.1643-15
8.1643-15
   O2                      0.0        0.0        0.0        0.0
0.0
   PALLA-01                0.0        0.0        0.0        0.0
0.0
 TOTAL FLOW:
   LBMOL/HR             1253.0544  1233.3382  1233.3382  1175.1204
1175.1204
   LB/HR                1.1220+05  1.1164+05  1.1164+05  1.1058+05
1.1058+05
   CUFT/HR              2.3654+05  1645.2789  1645.4256  1924.8767
1926.1905
 STATE VARIABLES:
   TEMP   F               77.0000    77.0000    77.2014   379.6558
380.7029
   PRES   PSIA             0.4834     0.4834    20.3053    19.8504
145.0377
   VFRAC                1.5735-02     0.0        0.0        0.0
0.0
   LFRAC                   0.9843     1.0000     1.0000     1.0000
1.0000
   SFRAC                   0.0        0.0        0.0        0.0
0.0
 ENTHALPY:
   BTU/LBMOL           -6.8630+04 -6.8904+04 -6.8896+04 -5.1655+04 -
5.1595+04
   BTU/LB               -766.4665  -761.2101  -761.1233  -548.9220  -
548.2918
   BTU/HR              -8.5998+07 -8.4982+07 -8.4972+07 -6.0701+07 -
6.0631+07
 ENTROPY:
   BTU/LBMOL-R           -78.3855   -80.0427   -80.0282   -61.3250   -
61.2550
   BTU/LB-R               -0.8754    -0.8843    -0.8841    -0.6517    -
0.6509
```

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STREAM SECTION

S13 S14 S15 S16 S17 (CONTINUED)

STREAM ID	S13	S14	S15	S16	S17
DENSITY:					
LBMOL/CUFT	5.2975-03	0.7496	0.7496	0.6105	0.6101
LB/CUFT	0.4743	67.8551	67.8491	57.4485	57.4093
AVG MW	89.5412	90.5190	90.5190	94.1021	94.1021

```
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                                  STREAM SECTION

 S18 S19 S2 S20 S3
 -----------------

 STREAM ID               S18         S19         S2          S20
S3
 FROM :                  C4          D1          F1          P4
C1
 TO   :                  R1          P4          C1          C3
S1

 SUBSTREAM: MIXED
 PHASE:                  LIQUID      LIQUID      VAPOR       LIQUID
MIXED
 COMPONENTS: LBMOL/HR
   PHENOL              1174.9518      2.6662      0.9734      2.6662
0.9734
   WATER                  0.1686  9.4323-26      2.2982  9.4323-26
2.2982
   DPC                    0.0        59.5188  1.9167-06    59.5188
1.9167-06
   CO                3.2232-11      0.0       549.4313      0.0
549.4313
   O2                     0.0         0.0         0.0         0.0
0.0
   PALLA-01               0.0         0.0         0.0         0.0
0.0
 COMPONENTS: MOLE FRAC
   PHENOL                 0.9999  4.2875-02  1.7612-03  4.2875-02
1.7612-03
   WATER             1.4347-04  1.5168-27  4.1581-03  1.5168-27
4.1581-03
   DPC                    0.0         0.9571  3.4679-09      0.9571
3.4679-09
   CO                2.7428-14      0.0         0.9941      0.0
0.9941
   O2                     0.0         0.0         0.0         0.0
0.0
   PALLA-01               0.0         0.0         0.0         0.0
0.0
 COMPONENTS: LB/HR
   PHENOL            1.1058+05    250.9246    91.6104    250.9246
91.6104
   WATER                  3.0372  1.6993-24    41.4022  1.6993-24
41.4022
   DPC                    0.0      1.2750+04  4.1058-04  1.2750+04
4.1058-04
```

```
   CO                  9.0282-10     0.0     1.5390+04     0.0
1.5390+04
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0        0.0        0.0        0.0
0.0
 COMPONENTS: MASS FRAC
   PHENOL                 1.0000  1.9301-02  5.9017-03  1.9301-02
5.9017-03
   WATER               2.7466-05  1.3071-28  2.6672-03  1.3071-28
2.6672-03
   DPC                    0.0        0.9807  2.6450-08     0.9807
2.6450-08
   CO                  8.1643-15     0.0        0.9914     0.0
0.9914
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0        0.0        0.0        0.0
0.0
 TOTAL FLOW:
   LBMOL/HR            1175.1204    62.1850   552.7029    62.1850
552.7029
   LB/HR               1.1058+05  1.3000+04  1.5523+04  1.3000+04
1.5523+04
   CUFT/HR             1732.6440   193.0912  2.5996+04   193.1255
2.1869+04
 STATE VARIABLES:
   TEMP   F             194.0000   401.3933   176.0000   401.7180
77.0000
   PRES   PSIA          145.0377     1.0124   145.0377    19.5000
145.0377
   VFRAC                  0.0        0.0        1.0000     0.0
0.9964
   LFRAC                  1.0000     1.0000     0.0        1.0000
3.6047-03
   SFRAC                  0.0        0.0        0.0        0.0
0.0
 ENTHALPY:
   BTU/LBMOL          -6.1178+04 -1.7353+05 -4.7050+04 -1.7350+05 -
4.7820+04
   BTU/LB              -650.1238  -830.0401 -1675.2428  -829.8845 -
1702.6821
   BTU/HR             -7.1892+07 -1.0791+07 -2.6004+07 -1.0789+07 -
2.6430+07
 ENTROPY:
   BTU/LBMOL-R          -74.0244  -263.6229    17.7838  -263.5852
16.4662
   BTU/LB-R              -0.7866    -1.2610     0.6332    -1.2608
0.5863
```

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STREAM SECTION

S18 S19 S2 S20 S3 (CONTINUED)

STREAM ID	S18	S19	S2	S20	S3
DENSITY:					
LBMOL/CUFT	0.6782	0.3220	2.1261-02	0.3220	2.5273-02
LB/CUFT	63.8223	67.3280	0.5971	67.3161	0.7098
AVG MW	94.1021	209.0608	28.0853	209.0608	28.0853

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STREAM SECTION

S4 S5 S6 S7 S8

STREAM ID	S4	S5	S6	S7	S8
FROM :	S1	F1	V1	F2	S2
TO :	R1	V1	F2	S2	P1
SUBSTREAM: MIXED					
PHASE:	MIXED	LIQUID	MIXED	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
PHENOL	0.9247	1178.4683	1178.4683	0.4037	0.3996
WATER	2.1833	59.5771	59.5771	1.0552-04	1.0446-04
DPC	1.8209-06	60.1146	60.1146	0.5958	0.5898
CO	521.9597	18.0790	18.0790	1.1733-07	1.1616-07
O2	0.0	0.0	0.0	0.0	0.0
PALLA-01	0.0	0.3645	0.3645	0.3645	0.3609
COMPONENTS: MOLE FRAC					
PHENOL	1.7612-03	0.8951	0.8951	0.2959	0.2959
WATER	4.1581-03	4.5251-02	4.5251-02	7.7352-05	7.7352-05
DPC	3.4679-09	4.5659-02	4.5659-02	0.4368	0.4368
CO	0.9941	1.3732-02	1.3732-02	8.6014-08	8.6014-08
O2	0.0	0.0	0.0	0.0	0.0
PALLA-01	0.0	2.7686-04	2.7686-04	0.2672	0.2672
COMPONENTS: LB/HR					
PHENOL	87.0298	1.1091+05	1.1091+05	37.9921	37.6122
WATER	39.3321	1073.2988	1073.2988	1.9009-03	1.8819-03
DPC	3.9005-04	1.2877+04	1.2877+04	127.6269	126.3506

```
   CO                  1.4620+04   506.3994   506.3994  3.2865-06
3.2537-06
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0       64.6373    64.6373    64.6373
63.9909
 COMPONENTS: MASS FRAC
   PHENOL              5.9017-03     0.8842     0.8842     0.1650
0.1650
   WATER               2.6672-03  8.5569-03  8.5569-03  8.2555-06
8.2555-06
   DPC                 2.6450-08     0.1027     0.1027     0.5543
0.5543
   CO                     0.9914  4.0373-03  4.0373-03  1.4273-08
1.4273-08
   O2                     0.0        0.0        0.0        0.0
0.0
   PALLA-01               0.0     5.1532-04  5.1532-04     0.2807
0.2807
 TOTAL FLOW:
   LBMOL/HR             525.0677  1316.6036  1316.6036     1.3641
1.3505
   LB/HR               1.4747+04  1.2543+05  1.2543+05   230.2582
227.9556
   CUFT/HR             2.0776+04  1949.2275  5.5936+06     3.3358
3.3024
 STATE VARIABLES:
   TEMP   F              77.0000   176.0000   134.6026   248.0000
248.0001
   PRES   PSIA          145.0377   145.0377     0.1450     0.1450
0.1450
   VFRAC                  0.9964     0.0     9.6591-02     0.0
0.0
   LFRAC               3.6047-03     1.0000     0.9034     1.0000
1.0000
   SFRAC                  0.0        0.0        0.0        0.0
0.0
 ENTHALPY:
   BTU/LBMOL          -4.7820+04 -7.0751+04 -7.0751+04 -6.7997+04 -
6.7997+04
   BTU/LB             -1702.6821  -742.6476  -742.6476  -402.8307  -
402.8307
   BTU/HR             -2.5109+07 -9.3151+07 -9.3151+07 -9.2755+04 -
9.1828+04
 ENTROPY:
   BTU/LBMOL-R           16.4662   -81.2950   -80.8859   -59.2752   -
59.2752
   BTU/LB-R               0.5863    -0.8533    -0.8490    -0.3512    -
0.3512
```

STREAM SECTION

S4 S5 S6 S7 S8 (CONTINUED)

STREAM ID	S4	S5	S6	S7	S8
DENSITY:					
LBMOL/CUFT	2.5273-02	0.6754	2.3538-04	0.4089	0.4089
LB/CUFT	0.7098	64.3489	2.2424-02	69.0274	69.0274
AVG MW	28.0853	95.2684	95.2684	168.7978	168.7978

```
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                                 STREAM SECTION

 S9
 --

 STREAM ID                S9
 FROM :                   P1
 TO   :                   R1

 SUBSTREAM: MIXED
 PHASE:                   LIQUID
 COMPONENTS: LBMOL/HR
   PHENOL                  0.3996
   WATER                1.0446-04
   DPC                     0.5898
   CO                   1.1616-07
   O2                      0.0
   PALLA-01                0.3609
 COMPONENTS: MOLE FRAC
   PHENOL                  0.2959
   WATER                7.7352-05
   DPC                     0.4368
   CO                   8.6014-08
   O2                      0.0
   PALLA-01                0.2672
 COMPONENTS: LB/HR
   PHENOL                 37.6122
   WATER                1.8819-03
   DPC                   126.3506
   CO                   3.2537-06
   O2                      0.0
   PALLA-01               63.9909
 COMPONENTS: MASS FRAC
   PHENOL                  0.1650
   WATER                8.2555-06
   DPC                     0.5543
   CO                   1.4273-08
   O2                      0.0
   PALLA-01                0.2807
 TOTAL FLOW:
   LBMOL/HR                1.3505
   LB/HR                 227.9556
   CUFT/HR                 3.3112
 STATE VARIABLES:
   TEMP   F              252.7765
   PRES   PSIA           203.0528
   VFRAC                   0.0
   LFRAC                   1.0000
   SFRAC                   0.0
```

```
 ENTHALPY:
   BTU/LBMOL          -6.7686+04
   BTU/LB              -400.9909
   BTU/HR             -9.1408+04
 ENTROPY:
   BTU/LBMOL-R          -58.8333
   BTU/LB-R              -0.3485
```

STREAM SECTION

S9 (CONTINUED)

STREAM ID	S9
DENSITY:	
LBMOL/CUFT	0.4079
LB/CUFT	68.8444
AVG MW	168.7978

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PHYSICAL PROPERTY TABLES SECTION

TERDIAGRAM CURVE TABLE:TERDI-1

*** PHASE ENVELOPE RESULTS ***

LIQUID MOLE FRACTION

	PHENOL	WATER	DPC
1	0.0000	0.13280	0.86720
2	0.12499	0.24461	0.63040
3	0.18533	0.29522	0.51945
4	0.24179	0.33732	0.42089
5	0.29483	0.37444	0.33073
6	0.34209	0.41040	0.24751
7	0.37817	0.45090	0.17093
8	0.39210	0.50550	0.10240
9	0.36174	0.59275	0.45506E-01
10	0.35108	0.61044	0.38485E-01
11	0.33593	0.63316	0.30910E-01
12	0.30915	0.66929	0.21560E-01
13	0.24404	0.74666	0.92939E-02
14	0.21025	0.78382	0.59347E-02
15	0.18827	0.80734	0.43890E-02
16	0.17097	0.82559	0.34375E-02
17	0.88259E-01	0.91076	0.98180E-03
18	0.45948E-01	0.95353	0.51733E-03
19	0.24205E-01	0.97539	0.40755E-03
20	0.12850E-01	0.98675	0.39824E-03
21	0.68123E-02	0.99276	0.42622E-03
22	0.35412E-02	0.99599	0.46661E-03
23	0.17017E-02	0.99779	0.50710E-03
24	0.0000	0.99944	0.56497E-03

*** TIELINE RESULTS ***

	LIQUID 1 MOLE FRACTION			LIQUID 2 MOLE FRACTION		
	PHENOL	WATER	DPC	PHENOL	WATER	DPC
1	0.000	0.9994	0.5650E-03	0.000	0.1328	0.8672

```
 2   0.1251       0.2447       0.6301    |  0.1705E-02   0.9978
0.5070E-03
 3   0.2404       0.3364       0.4232    |  0.6707E-02   0.9929
0.4271E-03
 4   0.3485       0.4161       0.2354    |  0.2667E-01   0.9729
0.4151E-03
 5   0.3617       0.5927       0.4551E-01|  0.1710       0.8256
0.3438E-02
```

*** VAPOR POINT RESULTS ***

VAPOR MOLE FRACTION

	PHENOL	WATER	DPC
1	0.0000	0.99759	0.24061E-02
2	0.79473E-03	0.99725	0.19516E-02
3	0.30470E-02	0.99573	0.12207E-02
4	0.10770E-01	0.98884	0.39263E-03
5	0.34994E-01	0.96498	0.21454E-04

PHYSICAL PROPERTY TABLES SECTION

TERDIAGRAM CURVE TABLE:TERDI-1 (CONTINUED)

*** AZEOTROPE RESULTS ***

	AZEOTROPE MOLE FRACTION			TEMPERATURE	
	PHENOL	WATER	DPC	F	PHASE
1	0.2205	0.000	0.7795	845.0	1 STABLE
2	0.000	0.9976	0.2406E-02	355.8	2 UNSTABLE

```
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                              PROBLEM STATUS SECTION

 BLOCK STATUS
 ------------


**************************************************************************
******
 *
*
 * Calculations were completed with warnings
*
 *
*
 * All Unit Operation blocks were completed normally
*
 *
*
 * All streams were flashed normally
*
 *
*
 * The following Convergence blocks were
*
 * completed with warnings:
*
 *   $OLVER01
*
 *
*
 * All Property Tables were completed normally
*
 *
*
 * Properties estimation was completed normally
*
 *
*

**************************************************************************
******
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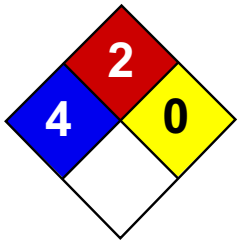
Appendix J: Material Safety Data Sheets



Material Safety Data Sheet
Phenol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Phenol

Catalog Codes: SLP4453, SLP5251

CAS#: 108-95-2

RTECS: SJ3325000

TSCA: TSCA 8(b) inventory: Phenol

CI#: Not available.

Synonym: Monohydroxybenzene; Benzenol; Phenyl hyroxide; Phenylic acid

Chemical Name: Carbolic Acid

Chemical Formula: C6H5OH

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Phenol	108-95-2	100

Toxicological Data on Ingredients: Phenol: ORAL (LD50): Acute: 317 mg/kg [Rat]. 270 mg/kg [Mouse]. DERMAL (LD50): Acute: 630 mg/kg [Rabbit]. 669 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (corrosive, irritant), of eye contact (irritant), of ingestion, of inhalation. Hazardous in case of skin contact (sensitizer, permeator). The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to kidneys, liver, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated

exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage. Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: 715°C (1319°F)

Flash Points: CLOSED CUP: 79°C (174.2°F). OPEN CUP: 85°C (185°F).

Flammable Limits: LOWER: 1.7% UPPER: 8.6%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances:
Flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards:
Phenol + nitrides results in heat and flammable gas generation. Phenol + mineral oxdizing acids results in fire. Phenol + calcium hypochlorite is an exothermic reaction producing toxic fumes which may ignite.

Special Remarks on Explosion Hazards:
Phenol + sodium nitrite causes explosion on heating. Peroxydisulfuric acid + phenol causes explosion.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Corrosive solid. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep container dry. Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Air Sensitive. Sensitive to light. Store in light-resistant containers. Moisture sensitive. Keep container tightly closed. Keep container in a cool, well-ventilated area.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 5 (ppm) from ACGIH (TLV) [United States] SKIN TWA: 19 (mg/m3) from ACGIH (TLV) [United States] SKIN TWA: 5 from NIOSH [United States] TWA: 19 (mg/m3) from NIOSH [United States] TWA: 5 (ppm) from OSHA (PEL) [United States] TWA: 19 (mg/m3) from OSHA (PEL) [United States] TWA: 5 (ppm) [Canada] TWA: 19 (mg/m3) [Canada]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor:
Distinct, aromatic, somewhat sickening sweet and acrid

Taste: Burning.

Molecular Weight: 94.11 g/mole

Color: Colorless to light pink

pH (1% soln/water): Not available.

Boiling Point: 182°C (359.6°F)

Melting Point: 42°C (107.6°F)

Critical Temperature: 694.2 (1281.6°F)

Specific Gravity: 1.057 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: 3.24 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.048 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 1.5

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol, diethyl ether, acetone.

Solubility:
Easily soluble in methanol, diethyl ether. Soluble in cold water, acetone. Solubility in water: 1g/15 ml water. Soluble in benzene. Very soluble in alcohol, chloroform, glycerol, petroleum, carbon disulfide, volatile and fixed oils, aqueous alkali hydroxides, carbon tetrachloride, acetic acid, liquid sulfur dioxide. Almost insoluble in petroleum ether. Miscible in acetone. Sparingly soluble in mineral oil.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources (flames, sparks), light, incompatible materials

Incompatibility with various substances: Reactive with oxidizing agents, metals, acids, alkalis.

Corrosivity:
Extremely corrosive in presence of copper. Slightly corrosive in presence of stainless steel(304), of stainless steel(316). Non-corrosive in presence of glass, of aluminum.

Special Remarks on Reactivity:
Air and light sensitive. Prone to redden on exposure to light and air. Incompatible with aluminum chloride, peroxydisulfuirc acid, acetaldehyde, sodium nitrite, boron trifluoride diethyl ether + 1,3-butadiene, isocyanates, nitrides, mineral oxidizing acids, calcium hypochlorite, halogens, formaldehyde, metals and alloys, lead, zinc, magnesium and their alloys, plastics, rubber, coatings, sodium nitrate + trifluoroacetic acid. Phenol + isocyanates results in heat generation, and violent polymerization. Phenol + 1,3-butadiene and boron trifluoride diethyl ether complex results in intense exothermic reaction. Phenol + acetaldehyde resultes in violent condensation.

Special Remarks on Corrosivity:
Minor corrosive effect on bronze. Severe corrosive effect on brass.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 270 mg/kg [Mouse]. Acute dermal toxicity (LD50): 630 mg/kg [Rabbit].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: kidneys, liver, central nervous system (CNS).

Other Toxic Effects on Humans:
Very hazardous in case of skin contact (corrosive, irritant), of ingestion, . Hazardous in case of skin contact (sensitizer, permeator), of eye contact (corrosive), of inhalation (lung corrosive).

Special Remarks on Toxicity to Animals:
Lowest Published Lethal Dose: LDL [Human] - Route: Oral; Dose: 140 mg/kg LDL [Infant] - Route: Oral; Dose: 10,000 mg/kg

Special Remarks on Chronic Effects on Humans:
Animal: passes through the placental barrier. May cause adverse reproductive effects and birth defects (teratogenic) Embryotoxic and/or foetotoxic in animal. May affect genetic material (mutagenic).

Special Remarks on other Toxic Effects on Humans:

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 125 mg/l 24 hours [Fish (Goldfish)]. >50 mg/l 1 hours [Fish (Fathead minnow)]. >50 mg/l 24 hours [Fish (Fathead minnow)]. >33 mg/l 72 hours [Fish (Fathead minnow)]. >33 ppm 96 hours [Fish (Fathead minnow)].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 6.1: Poisonous material.

Identification: : Phenol, solid UNNA: 1671 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Phenol Illinois toxic substances disclosure to employee act: Phenol Illinois chemical safety act: Phenol New York release reporting list: Phenol Rhode Island RTK hazardous substances: Phenol Pennsylvania RTK: Phenol Minnesota: Phenol Massachusetts RTK: Phenol Massachusetts spill list: Phenol New Jersey: Phenol New Jersey spill list: Phenol Louisiana RTK reporting list: Phenol Louisiana spill reporting: Phenol TSCA 8(b) inventory: Phenol TSCA 4(a) proposed test rules: Phenol TSCA 8(a) IUR: Phenol TSCA 8(d) H and S data reporting: Phenol: effective: 6/1/87; sunset:

6/01/97 SARA 302/304/311/312 extremely hazardous substances: Phenol SARA 313 toxic chemical notification and release reporting: Phenol CERCLA: Hazardous substances.: Phenol: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS D-1A: Material causing immediate and serious toxic effects (VERY TOXIC). CLASS D-2A: Material causing other toxic effects (VERY TOXIC). CLASS E: Corrosive solid.

DSCL (EEC):
R24/25- Toxic in contact with skin and if swallowed. R34- Causes burns. R40- Possible risks of irreversible effects. R43- May cause sensitization by skin contact. R52- Harmful to aquatic organisms. S1/2- Keep locked up and out of the reach of children. S24- Avoid contact with skin. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S28- After contact with skin, wash immediately with plenty of water S37/39- Wear suitable gloves and eye/face protection. S45- In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). S46- If swallowed, seek medical advice immediately and show this container or label. S56- Dispose of this material and its container at hazardous or special waste collection point.

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 2

Reactivity: 0

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 4

Flammability: 2

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 11:17 AM

Last Updated: 06/09/2012 12:00 PM

Material Safety Data Sheet

Oxygen

Section 1. Chemical product and company identification

Product name : Oxygen

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Molecular oxygen; Oxygen molecule; Pure oxygen; O2; Liquid-oxygen-; UN 1072; UN 1073; Dioxygen; Oxygen USP, Aviator's Breathing Oxygen (ABO)

MSDS # : 001043

Date of Preparation/Revision : **6/16/2011.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas.

Emergency overview : DANGER!

GAS:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
May cause severe frostbite.
LIQUID:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
Extremely cold liquid and gas under pressure.
May cause severe frostbite.

Do not puncture or incinerate container. Store in tightly-closed container. Avoid contact with combustible materials.

Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : May cause eye irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : May cause skin irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Respiratory system irritation after overexposure to high oxygen concentrations.

Ingestion : Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Oxygen	7782-44-7	100	

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : None expected.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : If inhaled, remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Non-flammable.

Products of combustion : No specific data.

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: reducing materials, combustible materials and organic materials.

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Contact with combustible material may cause fire. This material increases the risk of fire and may aid combustion. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Eliminate all ignition sources if safe to do so. Do not touch or walk through spilled material. Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Store in tightly-closed container. Avoid contact with combustible materials. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

Storage : Keep container tightly closed. Keep container in a cool, well-ventilated area. Separate from acids, alkalies, reducing agents and combustibles. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name

Oxygen

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 32 g/mole

Molecular formula : O2

Boiling/condensation point : -183°C (-297.4°F)

Melting/freezing point : -218.4°C (-361.1°F)

Critical temperature : -118.6°C (-181.5°F)

Vapor density : 1.105 (Air = 1) Liquid Density@BP: 71.23 lb/ft3 (1141 kg/m3)

Specific Volume (ft^3/lb) : 12.0482

Gas Density (lb/ft^3) : 0.083

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials, reducing materials and combustible materials.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Environmental fate : Not available.

Environmental hazards : This product shows a low bioaccumulation potential.

Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).	 	**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 75 kg **Cargo aircraft** Quantity limitation: 150 kg **Special provisions** A52
TDG Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).	 	**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship**

						Index 50 **Passenger Carrying Road or Rail Index** 75 **Special provisions** 42
Mexico Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations :

TSCA 8(a) IUR: Partial exemption
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Oxygen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Oxygen: Fire hazard, Sudden release of pressure, Delayed (chronic) health hazard

State regulations :

Connecticut Carcinogen Reporting: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) :

Class A: Compressed gas.
Class C: Oxidizing material.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : GAS:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
May cause severe frostbite.
LIQUID:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
Extremely cold liquid and gas under pressure.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.
Class C: Oxidizing material.

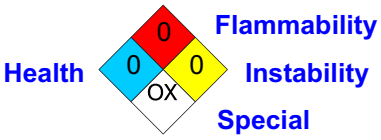
Hazardous Material Information System (U.S.A.) :

Health	0
Flammability	0
Physical hazards	0

liquid:

Health	3
Fire hazard	0
Reactivity	0
Personal protection	

National Fire Protection Association (U.S.A.) :



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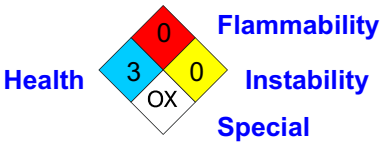


Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Material Safety Data Sheet

Carbon Monoxide

Section 1. Chemical product and company identification

Product name : Carbon Monoxide

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Carbon oxide (CO); CO; Exhaust Gas; Flue gas; Carbonic oxide; Carbon oxide; Carbone; Carbonio; Kohlenmonoxid; Kohlenoxyd; Koolmonoxyde; NA 9202; Oxyde de carbone; UN 1016; Wegla tlenek; Flue gasnide; Carbon monooxide

MSDS # : 001014

Date of Preparation/Revision : **12/3/2012.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [[COLORLESS GAS, MAY BE A LIQUID AT LOW TEMPERATURE OR HIGH PRESSURE.]]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Avoid breathing gas. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Toxic by inhalation.

Ingestion : Ingestion is not a normal route of exposure for gases

Potential chronic health effects

Chronic effects : May cause target organ damage, based on animal data.

Target organs : May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Carbon Monoxide	630-08-0	100	**ACGIH TLV (United States, 2/2010).** TWA: 29 mg/m³ 8 hour(s). TWA: 25 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 10 hour(s). TWA: 35 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 55 mg/m³ 8 hour(s). TWA: 50 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 8 hour(s). TWA: 35 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 605°C (1121°F)

Flammable limits : Lower: 12.5% Upper: 74.2%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

Product name

carbon monoxide

ACGIH TLV (United States, 2/2010).
TWA: 29 mg/m³ 8 hour(s).
TWA: 25 ppm 8 hour(s).
NIOSH REL (United States, 6/2009).
CEIL: 229 mg/m³
CEIL: 200 ppm
TWA: 40 mg/m³ 10 hour(s).
TWA: 35 ppm 10 hour(s).
OSHA PEL (United States, 6/2010).
TWA: 55 mg/m³ 8 hour(s).

TWA: 50 ppm 8 hour(s).
OSHA PEL 1989 (United States, 3/1989).
CEIL: 229 mg/m³
CEIL: 200 ppm
TWA: 40 mg/m³ 8 hour(s).
TWA: 35 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 28.01 g/mole
Molecular formula : C-O
Boiling/condensation point : -191°C (-311.8°F)
Melting/freezing point : -205°C (-337°F)
Critical temperature : -140.1°C (-220.2°F)
Vapor density : 0.97 (Air = 1)
Specific Volume (ft ^{3}/lb) : 13.8889
Gas Density (lb/ft ^{3}) : 0.072

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	Result	Species	Dose	Exposure
carbon monoxide	TDLo Intraperitoneal	Rat	35 mL/kg	-
	LC50 Inhalation Vapor	Rat	13500 mg/m3	15 minutes
	LC50 Inhalation Vapor	Rat	1900 mg/m3	4 hours
	LC50 Inhalation Gas.	Rat	6600 ppm	30 minutes
	LC50 Inhalation Gas.	Rat	3760 ppm	1 hours
	LC50 Inhalation Gas.	Mouse	2444 ppm	4 hours
	LC50 Inhalation Gas.	Rat	1807 ppm	4 hours

IDLH : 1200 ppm
Chronic effects on humans : **TERATOGENIC EFFECTS**: Classified 1 by European Union.
May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2).

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		Inhalation hazard zone D **Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 25 kg **Special provisions** 4
TDG Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0 **ERAP Index** 500 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index**

						Forbidden
Mexico Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: Not determined
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: carbon monoxide
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: carbon monoxide: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

California Prop. 65 : **WARNING:** This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

Ingredient name	Cancer	Reproductive	No significant risk level	Maximum acceptable dosage level
Carbon Monoxide	No.	Yes.	No.	No.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

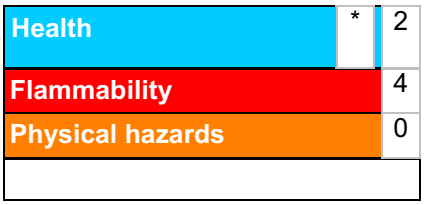
United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

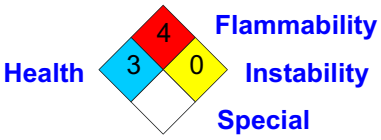
Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

Hazardous Material Information System (U.S.A.) :



National Fire Protection Association (U.S.A.) :



Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

MATERIAL SAFETY DATA SHEET

Date Printed: 03/03/2004
Date Updated: 09/02/2002
Version 1.1

Section 1 - Product and Company Information

Product Name	DIPHENYL CARBONATE, 99%
Product Number	D206539
Brand	ALDRICH
Company	Sigma-Aldrich
Street Address	3050 Spruce Street
City, State, Zip, Country	SAINT LOUIS MO 63103 US
Technical Phone:	314 771 5765
Emergency Phone:	414 273 3850 Ext. 5996
Fax:	800 325 5052

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
DIPHENYL CARBONATE	102-09-0	No

Formula	C13H10O3
Synonyms	Diphenyl carbonate * Phenyl carbonate * Phenyl carbonate ((PhO)2CO)
RTECS Number:	FG0500000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Harmful.
Harmful in contact with skin and if swallowed.
Possible sensitizer.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

Section 5 - Fire Fighting Measures

FLASH POINT

334.4 °F 168 °C Method: closed cup

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

EXTINGUISHING MEDIA
Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING
Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE(S) OF PERSONAL PRECAUTION(S)
Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP
Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING
User Exposure: Do not breathe dust. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE
Suitable: Keep tightly closed. Store in a cool dry place.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS
Safety shower and eye bath. Use only in a chemical fume hood.

PERSONAL PROTECTIVE EQUIPMENT
Other: Wear appropriate government approved respirator, chemical-resistant gloves, safety goggles, other protective clothing.

GENERAL HYGIENE MEASURES
Wash contaminated clothing before reuse. Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Color: White Form: Fine plates	
Property	Value	At Temperature or Pressure
Molecular Weight	214.22 AMU	
pH	N/A	
BP/BP Range	301 - 302 °C	760 mmHg
MP/MP Range	79 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	

VOC Content	N/A
Water Content	N/A
Solvent Content	N/A
Evaporation Rate	N/A
Viscosity	N/A
Surface Tension	N/A
Partition Coefficient	N/A
Decomposition Temp.	N/A
Flash Point	334.4 °F 168 °C Method: closed cup
Explosion Limits	N/A
Flammability	N/A
Autoignition Temp	N/A
Refractive Index	N/A
Optical Rotation	N/A
Miscellaneous Data	N/A
Solubility	N/A

N/A = not available

Section 10 - Stability and Reactivity

STABILITY
Stable: Stable.
Materials to Avoid: Strong oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS
Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION
Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE
Skin Contact: May cause skin irritation.
Eye Contact: May cause eye irritation.
Inhalation: Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.
Multiple Routes: Harmful if swallowed or absorbed through skin.

SENSITIZATION
Sensitization: Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

SIGNS AND SYMPTOMS OF EXPOSURE
Prolonged exposure can cause: Lung irritation. Dermatitis. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

TOXICITY DATA

Oral
Rat
1500 mg/kg
LD50
Remarks: Behavioral:Convulsions or effect on seizure threshold.

CHRONIC EXPOSURE - CARCINOGEN

Species: Mouse Mouse
Route of Application: Oral Oral
Dose: 28 GM/KG 28 GM/KG

Exposure Time: 78W 78W
Frequency: I I
Result: Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Lungs, Thorax, or Respiration:Tumors. Liver:Tumors. Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Lungs, Thorax, or Respiration:Tumors. Liver:Tumors.

Species: Mouse Mouse
Route of Application: Subcutaneous Subcutaneous
Dose: 1000 MG/KG 1000 MG/KG
Result: Tumorigenic:Neoplastic by RTECS criteria. Liver:Tumors. Tumorigenic:Neoplastic by RTECS criteria. Liver:Tumors.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION
Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT
Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA
Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION
Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22
Risk Statements: Harmful if swallowed.
S: 22 24/25
Safety Statements: Do not breathe dust. Avoid contact with skin and eyes.

US CLASSIFICATION AND LABEL TEXT
Indication of Danger: Harmful.
Risk Statements: Harmful in contact with skin and if swallowed.
Safety Statements: Wear suitable protective clothing.
US Statements: Possible sensitizer.

UNITED STATES REGULATORY INFORMATION
SARA LISTED: No
TSCA INVENTORY ITEM: Yes Yes

CANADA REGULATORY INFORMATION
WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes

NDSL: No

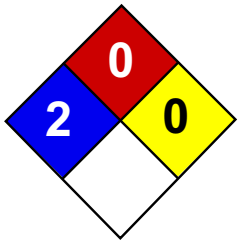
Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



Health	2
Fire	0
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Palladium chloride MSDS

Section 1: Chemical Product and Company Identification

Product Name: Palladium chloride

Catalog Codes: SLP1378

CAS#: 7647-10-1

RTECS: RT3500000

TSCA: TSCA 8(b) inventory: Palladium chloride

CI#: Not available.

Synonym: Palladium (II) Chloride

Chemical Name: Palladium Chloride

Chemical Formula: PdCl2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Palladium chloride	7647-10-1	100

Toxicological Data on Ingredients: Palladium chloride: ORAL (LD50): Acute: 2704 mg/kg [Rat]. >1000 mg/kg [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, sensitizer).

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.

Skin Contact:
Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system.

Section 7: Handling and Storage

Precautions:
Do not ingest. Do not breathe dust. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as metals, acids.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 24°C (75.2°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance:
Solid. (Amorphous solid powder or lumps. Deliquescent solid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 177.3 g/mole

Color: Red-Brown. (Dark.)

pH (1% soln/water): Not available.

Boiling Point: Not available.

Melting Point: 679°C (1254.2°F)

Critical Temperature: Not available.

Specific Gravity: 4 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, acetone.

Solubility: Soluble in cold water, acetone, hydrobromic acid.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat, moisture, incompatible materials

Incompatibility with various substances: Reactive with metals, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Incompatible with organic solvents, acids, NH3, Zn, strong oxidizing agents, aluminum, magnesium, nitrates, thiocyanates

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): >1000 mg/kg [Mouse].

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, sensitizer).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and cancer based on animal data. May affect genetic material

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. May affect metabolism if absorbed through skin. Eyes: Causes eye irritation. May cause chemical conjunctivitis. Ingestion: May cause gastrointestinal tract irritation with nausea, vomiting and diarrhea. May affect blood, immumological system, and metabolsim Inhalation: Causes respiratory tract and mucous membrane irritation.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Palladium chloride

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC):
R36- Irritating to eyes. S2- Keep out of the reach of children. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 0

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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